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RESEARCH ARTICLE

Effect of Different Parameters on Production of Rice Using Machine Learning

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ABSTRACT

Different parameters influence the production of rice. For the study, the effects of longitude, latitude, Rain (Jan-Dec), Rain (Nov-May), Rain (June-Oct), Temperature (Jan-Dec), Temperature(Nov-May), and Temperature(June-Oct) on production of rice was studied.“Pipeline Pilot module of Biovia software” (Dassault Systems of France) was used for analysis. The software provides different built-in components to develop a “machine learning model” and use the model for prediction.

Keywords: Neural network, Rice, Latitude, Longitude, Rain, Temperature.

INTRODUCTION

Machine Learning

The study of computer algorithms that improve automatically through experiment is called Machine Learning (ML). To develop data analysis that automates analytical model building the machine learning method is used. The “machine learning” is a branch of “artificial intelligence” based on the idea that systems can learn from the data, recognize patterns and make decisions with minimal human intervention. The machine learning today is not like machine learning of past because of new computing technologies. It was born out of pattern recognition and the theory that computers can learn to do certain works without being programmed; researchers interested in artificial intelligence want to see if computers can learn from the data. The iterative aspect of machine learning is important, because they can adapt independently as models are exposed to new data.

While many "machine learning algorithms" have been around for a long time, a recent breakthrough is the ability to automatically apply complex mathematical computations to big data-over and over, faster and faster. Here are a number of highly known examples of machine learning applications that we should know about:

- "The heavily hyped, self-driving Google car"?
  (The essence of machine learning)
- "Online recommendation offers such as those from Amazon, Netflix etc".?
  (The application of machine learning in everyday life)
- "The detection of Fraud"?
  (One of the more important uses in our world)
- "Get the idea that what customers are saying about us on Twitter"?
  (Combination of machine learning with linguistic rule creation)

As we know that "artificial intelligence" (AI) is a broad science of imitating human abilities, "machine learning" is a specific branch of AI that trains a computer to learn. The resurgent interest in "machine learning" stems from the same reasons that made "data mining" and "Bayesian analysis" more common than ever before. Many financial industry and banks companies use "machine learning technology" for two main purposes: finding valuable data trends and preventing fraud. The insights can identify opportunities to invest, or help investors know when to trade. "Data mining" may also identify high-risk clients or use cyber surveillance to detect fraud warning signs. Moreover the "machine learning and artificial intelligence" is useful in Health care, Oil and Gas, Transportation and many other Government sector.

Rice Production

The production of rice in India is an important part of national economy. The most prominent crop of India is rice so rice is the main food of most of the people in India. This crop is the back bone of the millions of people in India, and plays a vital role in the country's food security, so "rice is life" is the most prominent word in Indian context. So to get maximum production in rice many models and techniques are developed by using Machine Learning (ML) and Artificial Intelligence (AI).Machine learning in agriculture used to improve the productivity and quality of the crops in the agricultural field. The seed retailers use this technique to churn the data to create bettor crops, whereas the pest control industries are using them to identify the various bacteria's, bugs and vermins. Mainly agriculture uses AI technology to aid to find disease in crops, pests and poor plant nutrition on farms. Rice is a significant harvest used as a staple food across the world and especially in Asia. The production to develop rice is exceptionally human work escalated. A significant part of the troublesome work of rice creation can be mechanized with cleaver and automated stages.

REVIEW OF LITERATURE

Rice as a Crop

Rice, (Oryza sativa), edible starchy cereal grain, and the grass plant (Poaceae family) from which it is made. Approximately half of the world's population, including virtually all of East and Southeast Asia, relies heavily on rice as a staple food; 95 % of the world's rice crop is eaten by humans [1]. Rice is the most important human food crop in the world, directly feeding more people than any other crop. In 2012, nearly half of world's population – more than 3 billion people – relied on rice every day. It is also the staple food across Asia where around half of the world's poorest people live and is becoming increasingly important in Africa and Latin America [2]. "Rice is produced in a wide range of locations and under a variety of climatic conditions, from the wettest areas in the world to the driest deserts. It is produced along Myanmar's Arakan Coast, where the growing season records an average of more than 5,100 mm of rainfall, and at Al Hasa Oasis in Saudi Arabia, where annual rainfall is less than 100 mm. Temperatures, too, vary greatly. In the Upper Sind in Pakistan, the rice season averages 33 °C; in Otaru, Japan, the mean temperature for the growing season is 17 °C. The crop is produced at sea level on coastal plains and in delta regions throughout Asia, and to a height of 2,600 m on the slopes of Nepal's mountains" [3].

Productivity

"Global rice production more than tripled between 1961 and 2010, with a compound growth rate of 2.24% per year (2.21% in rice-producing Asia). This increase was slightly greater than that for wheat (2.02% per year), but substantially less than that for maize, which grew at 2.71% per year. Most of the increase in rice production was due to higher yields, which increased at an annual average rate of 1.74%, compared with an annual average growth rate of 0.49% for area harvested. In absolute terms, paddy yields increased at an annual average rate of 51.1 kg/ha per year, although this rate of increase has declined in both percentage and absolute terms" [4].

Half of the global human population is dependent on rice as a staple food crop and more than 25% increase in rice productivity is required to feed the global population by 2030.

Recent work done

There are plenty of research articles available in the field of rice production and the allied area of rice production. In the present section of this paper our objective is to provide an insight in the field of IT integration in agriculture (especially in rice production). Here are some important eye opener (few selected) recent articles which comprises of Machin Learning techniques (such as NN, ANN, PSO etc). Chen and Mcnairn [5] studied "A neural network integrated approach for rice crop monitoring". They have used neural network to predict the rice yield. Asada and Matsumoto [6] investigated "Effects of rainfall variation on rice production in the Ganges-Brahmaputra Basin". They have concentrated their study about the rice production in Ganges-Brahmaputra basin area. Gandhi et al [7] carried out a research study on "Rice crop yield prediction using artificial neural networks". They have used Support Vector Machine approach for the prediction. Liu et al [8] studied "Geographical Variation of Climate Change Impact on Rice Yield in the Rice-Cropping Areas of Northeast China during 1980–2008". Lu et al [9] have done a research study on "Identification of rice diseases using deep convolutional neural networks". Maeda et al [10], studied "Yield Prediction of Paddy Rice with Machine Learning", Recently Zhang et al [11] investigated "Mapping Rice Paddy Based on Machine Learning with Sentinel-2 Multi-Temporal Data: Model Comparison and Transferability". Coming forward in the similar direction, many researchers [12-21], concentrated their studies to get some insights into the production of rice using different methods into consideration.

Objectives

To determine the effect of parameters on production of Rice using machine learning. In this study we can determine the suitable condition where the rice grows in a manner that we can get maximum profit.

MATERIALS AND METHODS

Software used

"Pipeline Pilot module of Biovia software" (DassaultSystems of France) is used for analysis. The software provides different built-in components to develop a "machine learning model" and use the model for prediction.

Methodology

Collection of data

Data was collected from website. Longitude, latitude, Temperature (Jan-Dec), Temperature (Nov-May), Temperature (June-Oct), Rain (Jan-Oct), Rain (Nov-May), Rain (June-Oct) were taken as input while production of rice was used as output parameter.

Development of deep learning neural network model

The dataset was read using "Delimited Text Reader" component of "pipeline pilot". The component was connected to the "Learn R Deep Neural Net Model" component. The output of the model was displayed using "HTML Table Viewer" component. The parameters for the "Learn R Deep Neural Net Model" component were set as shown in

Figure 1. The setting for which the experimental output parameter and the predicted parameter were close to a 45^0 line were considered for the final model.

Study of effect of different input parameters on rice production

Text files were prepared where one parameter was varied within the range of data analyzed. All other parameters were kept constant at an average value.

RESULTS AND DISCUSSION

Rice production varies due to different reasons. However, the relationships are difficult to predict. Thus, this study focuses on the effect of various input parameters on the rice production.

Prediction ability of the model

Figure 2a shows the model developed. Figure 2b shows that the prediction ability of the model was good and the predictions were close to the experimental values.

Prediction by the model

Figure 3 shows that the rice production in the particular area is gradually increasing after the longitude crossed 80^oE, while the production of rice is minimum in between longitude 0^oE to 80^oE. The results showed that high value of longitude favored rice production. Figure 4 shows that the production of rice is gradually decreasing if the latitude exceeds 15^o N while the production is increasing if the latitude is in between 0^oN to 15^o N. The analysis shows that rice production is high at around 15^oN. Figure 5 indicates that the production of rice in gradually increasing when the rain amount in the month June-October exceeds 250mm. The production of crop is minimum when the rain is in between around 250mm. The production of rice is very high if the rainfall during June-October is high (around 600 mm).

Figure 6 shows that the rice production is gradually decreasing in the month November-May when the rain amount exceeds 40mm .And the rice production is in the pick if the rain amount is between 0 mm to 40mm. Figure 7 represents that the production of rice is directly proportional to the temperature in the month January-December. But after the temperature 25^0C it starts slow decrease. So the maximum productivity of rice in Jan-Dec is in 25^oC. Figure 8 shows that the production of rice is gradually increasing when the temperature is increasing in November-May and after the temperature exceeds 23^oC the production rate is constant. Figure 9 indicates that the production of rice is inversely proportional to the temperature in June-October i.e. the rice production is gradually decreasing when the temperature is increasing in June-October. Figure 10 shows that the production of rice is gradually decreasing if the rain is increasing in between January-December. The production of rice is maximum when the amount of the rain is minimum in January-December. So the figure shows that the productivity of rice is maximum when the amount of rain is 50mm in between Jan-Dec.

CONCLUSIONS

The effects of different parameters on rice production have been studied using Pipeline pilot. The results shown that rice production is high at high values of longitude (above 80^o E), latitude (at 15^0 N), 600mm rain in June-Oct, 40mm rainin Nov-May, 50mm rain in Jan-Dec, 10^oC temperature in June-Oct, 23^oC temperature in Nov-May and 23^oC temperature in Jan-Dec.

REFERENCES

1. ENCYCLOPÆDIA BRITANNICA, https://www.britannica.com/plant/rice
2. Ricepedia, http://ricepedia.org/
3. Rice Almanac, 3rd edition, 2002, Edited by Maclean, J.L., Dawe, D.C., Hardy, B., and Hettel, G.P., CABI Publishing, UK.
4. Brady, N. C., "Soil Factors that Influence Rice Production", Proceedings of Symposium on Paddy Soils, 1981.
5. C. Chen and H. Mcnairn "A neural network integrated approach for rice crop monitoring", International Journal of Remote Sensing, Vol. 27, No. 7, (2006), pp. 1367–1393.
6. Haruhisa Asada and Jun Matsumoto, "Effects of rainfall variation on rice production in the Ganges-Brahmaputra Basin", CLIMATE RESEARCH, Vol. 38: 249–260, 2009, doi: 10.3354/cr00785
7. N. Gandhi, O. Petkar and L. J. Armstrong, "Rice crop yield prediction using artificial neural networks," 2016 IEEE Technological Innovations in ICT for Agriculture and Rural Development (TIAR), Chennai, 2016, pp. 105-110, doi: 10.1109/TIAR.2016.7801222.
8. Liu Z, Zhang G, Yang P., "Geographical Variation of Climate Change Impact on Rice Yield in the Rice-Cropping Areas of Northeast China during 1980–2008", Sustainability, 2016; 8(7):670, https://doi.org/10.3390/su8070670.
9. Lu, Y., Yi, S., Zeng, N., Liu, Y., Zhang, Y., "Identification of rice diseases using deep convolutional neural networks", Neurocomputing 267, (2017), 378-384.
10. Yuichiro Maeda, Taichi Goyodani, Shunsaku Nishiuchi and Eisuke Kita, "Yield Prediction of Paddy Rice with Machine Learning", Int'l Conf. Par. and Dist. Proc. Tech. and Appl., (PDPTA'18), (2018), pp. 361-365.
11. Weichun Zhang, Hongbin Liu, Wei Wu, Linqing Zhan and Jing Wei, "Mapping Rice Paddy Based on Machine Learning with Sentinel-2 Multi-Temporal Data: Model Comparison and Transferability", Remote Sensing, 12, (2020), pp. 1620; doi:10.3390/rs12101620.
12. Casanova, D., Goudriaan, J., Forner, M.C., Withagen, J., "Rice yield prediction from yield components and limiting factors", Eur. J. Agron., vol. 17, (2002), pp. 41–61.
13. Ali, A.M., Thind, H.S., Sharma, S., Varinderpalsingh, "Prediction of dry direct seeded rice yields using chlorophyll meter, leaf color chart and green seeker optical sensor in northwestern India", Field Crops Res., vol. 161, (2014), pp. 11–15.
14. Zhao, S., Zheng, H., Chi, M., Chai, X., Liu, Y., "Rapid yield prediction in paddy fields based on 2d image modelling of rice panicles", Comput. Electron. Agric. vol. 162, (2019), pp. 759–766.
15. Chun, J.A., Kim, S., Lee, W.S., Oh, S.M., Lee, H., "Assessment of multimodel ensemble seasonal hindcasts for satellite-based rice yield prediction", J. Agric. Meteorol. 72, (2016), pp. 107–115.
16. Das, B., Nair, B., Reddy, V.K., Venkatesh, P., "Evaluation of multiple linear, neural network and penalised regression models for prediction of rice yield based on weather parameters for west coast of india. Int. J. Biometeorol. vol. 62, (2018), pp. 1809–1822.
17. Dhekale, B., Nageswararao, M., Nair, A., Mohanty, U., Swain, D., Singh, K., Arunbabu, T., "Prediction of kharif rice yield at kharagpur using disaggregated extended range rainfall forecasts". Theoret. Appl. Climatol., vol. 133, (2018), pp. 1075–1091.
18. Jha, P.K., Athanasiadis, P., Gualdi, S., Trabucco, A., Mereu, V., Shelia, V., Hoogenboom, G., "Using daily data from seasonal forecasts in dynamic crop models for yield prediction: a case study for rice in nepal's terai", Agric. Forest Meteorol., vol. 265, (2019), pp. 349–358.
19. Ji, B., Sun, Y., Yang, S., Wan, J., "Artificial neural networks for rice yield prediction in mountainous regions", J. Agric. Sci., vol. 145, (2007), pp. 249–261.
20. Kandiannan, K., Karthikeyan, R., Krishnan, R., Kailasam, C., Balasubramanian, T., "A crop–weather model for prediction of rice (oryza sativa l.) yield using an empirical statistical technique, J. Agron. Crop Sci., vol. 188, (2002), pp. 59–62.
21. Koide, N., Robertson, A.W., Ines, A.V., Qian, J.H., DeWitt, D.G., Lucero, A., "Prediction of rice production in the philippines using seasonal climate forecasts", J. Appl. Meteorol. Climatol., vol. 52, (2013), pp. 552–569.

22. Siddique, M. and Panda, D. (2019) Prediction of Stock Index of Tata Steel using Hybrid Machine Learning Based Optimization Techniques, International Journal of Recent Technology and Engineering, Vol. 8 (2): 3186-3193.
23. Siddique, M. and Panda, (2019) D. A hybrid forecasting model for prediction of stock index of Tata Motors using principal component analysis, support vector regression and particle swarm optimization, International Journal of Engineering and Advanced Technology, Vol. 1 (9): 3032-3037.

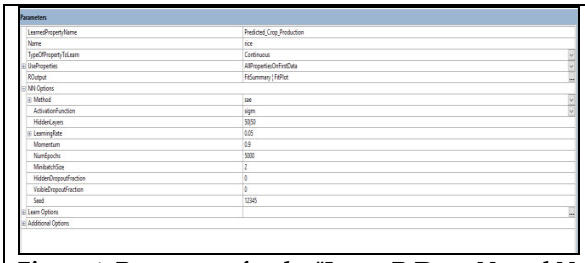

Figure 1. Parameters for the "Learn R Deep Neural Net Model" component

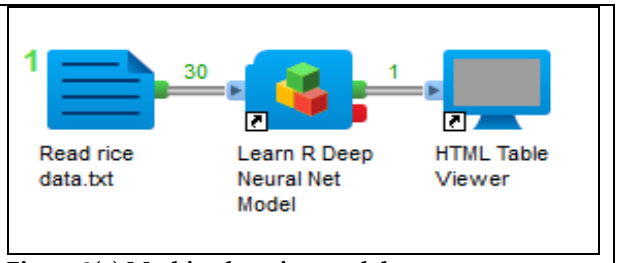

Figure 2(a) Machine learning model

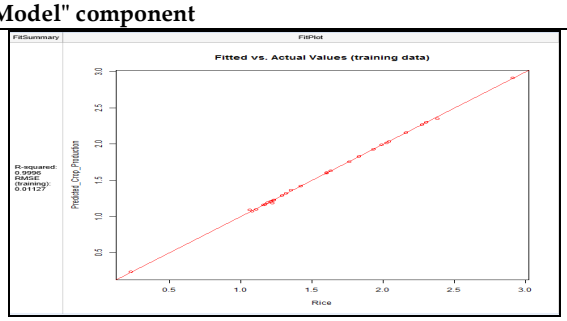

Figure 2 (b) Prediction capability of the model

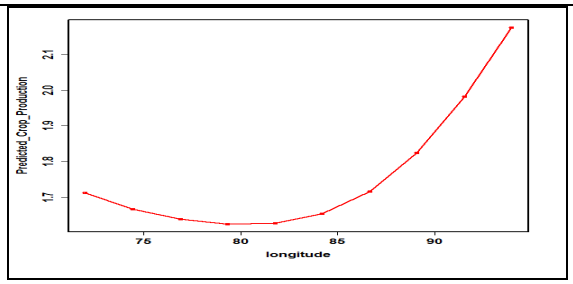

Figure 3: Effect of longitude in the production of Rice

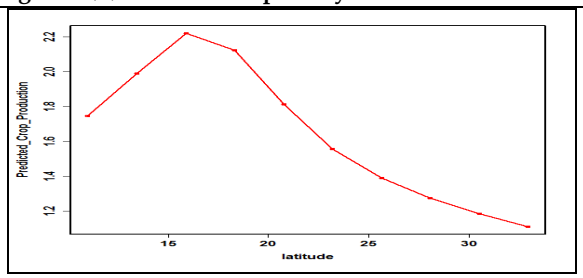

Figure 4: Effect of Latitude in the production of Rice

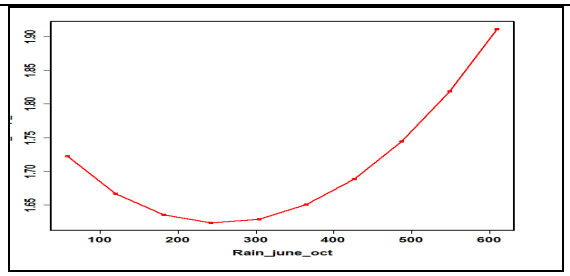

Figure 5: Effect of Rain in Jun-Oct in the production of Rice

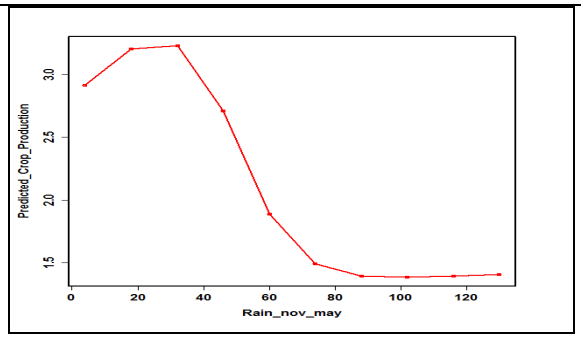

Figure 6: Effect of Rain in Nov-May in the production of Rice

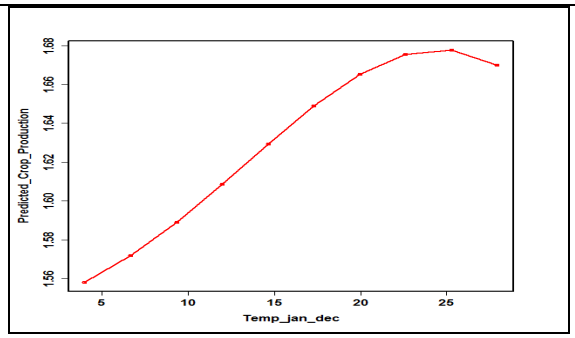

Figure 7: Effect of temperature in Jan-Dec in the production of Rice

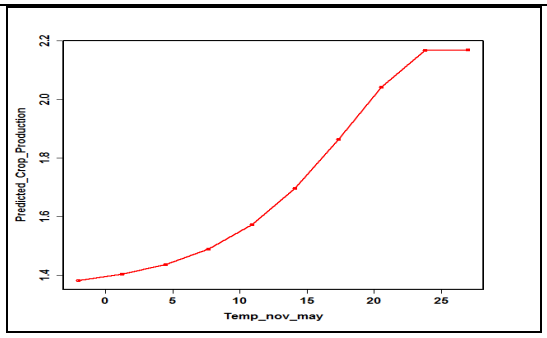

Figure 8: Effect of temp in Nov-May in the production of Rice

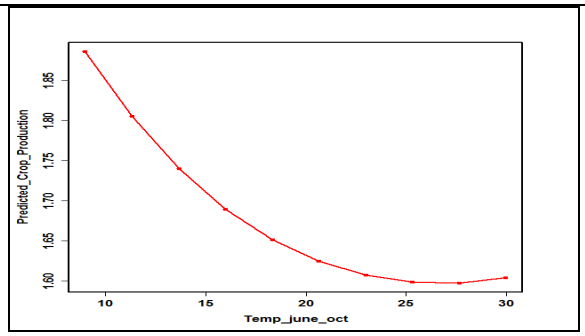

Figure 9: Effect of temp in June-Oct in the production of rice

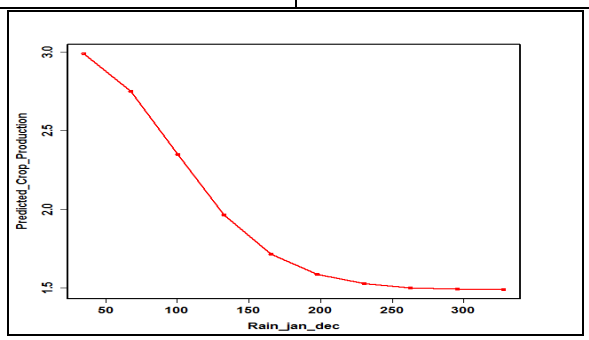

Figure 10: Effect of rain in Jan-Dec in the production of Rice

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RESEARCH ARTICLE

Effect of Different Parameters on Production of Sugarcane using Machine Learning

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ABSTRACT

Different parameters influence the production of sugarcane. For the study, the effects of longitude, latitude, Rain (Jan-Dec), Rain (Nov-May), Rain (June-Oct), Temperature (Jan-Dec), Temperature (Nov-May), and Temperature (June-Oct) on production of sugarcane was studied. Pipeline Pilot module of Biovia software (Dassault Systemes of France) was used for analysis. The software provides different built-in components to develop a machine learning model and use the model for prediction.

Keywords: Neural Network, Sugarcane, Latitude, Longitude, Rain, Temperature.

INTRODUCTION

Sugarcane as a Crop

"Sugarcane is one of the main perennial crop grown in tropical areas of various countries like India, Brazil, Thailand, China, Pakistan, Mexico etc. FAO suggested that more than 90 countries are cultivating sugarcane within the area of 26 million hector where the global harvest is 1.83 billion tons (FAO [1]). India is the second largest producer of sugarcane crop and produces about 20% of the world's sugarcane. It is one of the staple foods that are used in different countries. It is the raw material of mostly used food and other materials like bread, beverage & single cell protein (Pezhman et al. [2])". In view of worldwide environment, sugarcane is a significant resource of alcohol to convert into biofuels for motor vehicle and electricity generation. Simplified models for the prediction of growth of crop are capable of effective implementation of estimation of models for land use susceptibility (Adam et al. [3]). Such systems consider uptake of water through roots, succeeding loss through transpiration & their impact on growth. Several factors like daily growth (G), daily irrigation water (I), electric soil conductivity (EC), temperature (T), daily evaporation (E), wind speed (W), daily sun shine hours (S), humidity (H) are considered in different studies.

Machine Learning

BIOVIA Machine Learning provides a comprehensive range of capabilities for learning and data processing, statistical filters and clustering modules designed for massive data sets in the real world.

BIOVIA Machine Learning Features

Main features of BIOVIA Machine Learning are listed below:

i. Quickly combine data
ii. Use Bayesian statistics to employ categorical learning
iii. Conduct key component analysis (PCA)
iv. Apply regression-Linear, partial least squares (PLS) and neighbor k-nearest (kNN)
v. Using Recursive Partitioning methods to construct models of single tree or forest. The methods may be used to create models for single or multiple responses.
vi. Analyze vector value to classify the descriptors which are most selective
vii. Deploy Domain Applicability Model (MAD) methods and allow cross-validation to assess the quality of predictions
viii. Instead of a single "best" model, return multiple models by creating a number of trial models. Combine several models into one built model
ix. Employ Genetic Function Approximation (GFA) methods to perform variable selection and build multiple models, which may be combined into a consensus or ensemble model
x. Employ Pareto Optimization for multi-objective optimization problems
xi. Generate interactive reports with ROC plots, enrichment plots and other visualization techniques for evaluating model quality and understanding the relationships between descriptors and responses.
xii. Integrate with other statistic platforms like R, JMP and SAS.

Sugarcane production

The annual growing season covers the year of entry and is related to crops with yearlong growth cycle, such as sugarcane. Sugarcane is an important land-based cash or income crop.

REVIEW OF LITERATURE

Many researchers have done their research work in the area of the production of sugarcane. Few of them are listed below: Bahraniet al. [4] studied“Sugarcane responses to irrigation andnitrogen in subtropical Iran”.Barzegar et al[5] carried out a research study on“Effectiveness of sugarcane residue incorporation at different water contentsand the proctor compaction loads in reducing soilcompactibility”.Dashtegol et al [6] investigated“Effects of every-other furrow irrigation on water use efficiency and sugarcane characteristics in southern Ahvaz sugarcane fields”.Hamdi et al [7] have done an study on“Advances in TAE Sugarcane Breeding Program in Iran”.Karimi et al [8] studied “Energy analysis of sugarcane production in plant farms a case study in DebelKhazai agro-industry in Iran”.

Objectives

Objective of the present study is to determine the effect of various parameters on production of sugarcane using machine learning. In this study we can determine the suitable condition where the sugarcane grows in a manner that we can get maximum profit.

MATERIALS AND METHODS

Software used

“Pipeline Pilot module of Biovia software” (Dassault Systems of France) is used for analysis. The software provides different built-in components to develop a “machine learning model” and use the model for prediction.

Methodology

Collection of data

Data was collected from website. Longitude, Latitude, Temperature (Jan-Dec), Temperature (Nov-May), Temperature (June-Oct), Rain (Jan-Oct), Rain (Nov-May), Rain (June-Oct) were taken as input while production of sugarcane was used as output parameter.

Development of deep learning neural network model

The dataset was read using "Delimited Text Reader" component of pipeline pilot. The component was connected to the "Learn R Deep Neural Net Model" component. The output of the model was displayed using "HTML Table Viewer" component. The parameters for the "Learn R Deep Neural Net Model" component were set as shown in Figure 1. The setting for which the experimental output parameter and the predicted parameter were close to a 45^0 line were considered for the final model.

Study of effect of different input parameters on Sugarcane production

Text files were prepared where one parameter was varied within the range of data analysed. All other parameters were kept constant at an average value.

RESULTS AND DISCUSSION

Sugarcane production varies due to different reasons. However, the relationships are difficult to predict. Thus, this study focuses on the effect of various input parameters on the sugarcane production.

Prediction ability of the model

Figure 2a shows the model developed.Figure 2b shows that the prediction ability of the model was good and the predictions were close to the experimental values.

Prediction by the model

Figure 3 shows that the sugarcane production in the particular area is gradually increasing from 0°E to 85°E then it is decreasing after longitude crossed 85°E to 90°E. Then it is increasing after longitude crossed 90°E. Figure 4 shows that the production of sugarcanein the particulararea is gradually decreasing from 0°N to 30°N. Figure 5 indicates that the production of sugarcane is increases highly when the rainfall is in between 125 mm to 300 mm during the month June-October. The production of sugarcane is very high if the rainfall during June-October is high (around 600 mm). Figure 6 shows that the production of sugarcane in the particular area is gradually increasing, during the month Nov-May, when the rainfall increases from 0 mm to 110 mm. It is highest when the rainfall is around 120 mm. Figure 7 represents that the production of sugarcane in the particular area is gradually decreasing, during the month Jan-Dec, when temperature varies from 0°c to 25°c. Figure 8 shows that the production of sugarcane in the particular area is gradually decreasing when the temperature increases from 0°c to 30°c (during Nov-May). Figure 9 indicates that the production of sugarcane in the particular area is constantly increasing when the temperature increases from 0°c to 30°c (during June-Oct). Figure 10 shows that the production of sugarcane in particular area is gradually decreasing when the rainfall varies from 0 mm to 165 mm (during Jan-Dec) then it increases after crossed over around 160 mm.

CONCLUSIONS

The effects of different parameters on wheat production have been studied using Pipeline pilot. The results shows that wheat production is high at low values of longitude, latitude between 20°N to 25°N and low rainfall(100mm or less) , low temperature areas.

REFERENCES

1. WORLD AGRICULTURE TOWARDS 2030/2050, Food and Agriculture Organization of the United Nations (FAO) .2015.
2. PezhmanTahereiGhazvinei, Hossein HassanpourDarvishi, Amir Mosavi, Khamaruzaman bin Wan Yusof, MeysamAlizamir, ShahaboddinShamshirband& Kwok-wing Chau (2018), "Sugarcane growth prediction based on meteorological parameters using extreme learning machine and artificial neural network", Engineering Applications of Computational Fluid Mechanics, 12:1, 738-749, DOI: 10.1080/19942060.2018.1526119.
3. Adam M,EwertF,LeffelaarPA,CorbeelsM,VanKH,Wery Z.(2010). CROSPAL,software that uses agronomic expert knowledge to assist modules selections for crop growth stimulation. Environmental Modelling & Software. 25(8).946-955.
4. Bahrani, M., Shomeili, M., Zande-Parsa, S., &Kamgar-Haghighi, A. (2010). Sugarcane responses to irrigation and nitrogen in subtropical Iran.Iran Agricultural Research, 27–21. .2), pp. 17–26.
5. Barzegar, A., Asoodar, M., & Ansari, M. (2000). Effectiveness of sugarcane residue incorporation at different water contents and the proctor compaction loads in reducing soil compactibility. Soil and Tillage Research, 57(3), 167–172.
6. Dashtegol, A., Kashkooli, H., Naseri, A., &Nasab, S. (2009). Effects of every-other furrow irrigation on water use efficiency and sugarcane characteristics in southern Ahvaz sugarcane fields. Journal of Science and Technology of Agriculture and Natural Resources, 13(49 (B)), 45–58.
7. Hamdi, H., Baniabbasi,N., Almani,M.P.,&Babagoli, S. (2005). Advances in TAE Sugarcane Breeding Program in Iran. Proc. ISSCT.
8. Karimi, M., RajabiPour, A., Tabatabaeefar, A., &Borghei, A. (2008). Energy analysis of sugarcane production in plant farms a case study in DebelKhazai agro-industry in Iran. American-Eurasian Journal of Agricultural and Environmental Science, 4, 165–171.
9. Siddique, M. and Panda, D. (2019) Prediction of Stock Index of Tata Steel using Hybrid Machine Learning Based Optimization Techniques, International Journal of Recent Technology and Engineering, Vol. 8 (2): 3186-3193.
10. Siddique, M. and Panda, (2019) D. A hybrid forecasting model for prediction of stock index of Tata Motors using principal component analysis, support vector regression and particle swarm optimization, International Journal of Engineering and Advanced Technology, Vol. 1 (9): 3032-3037.

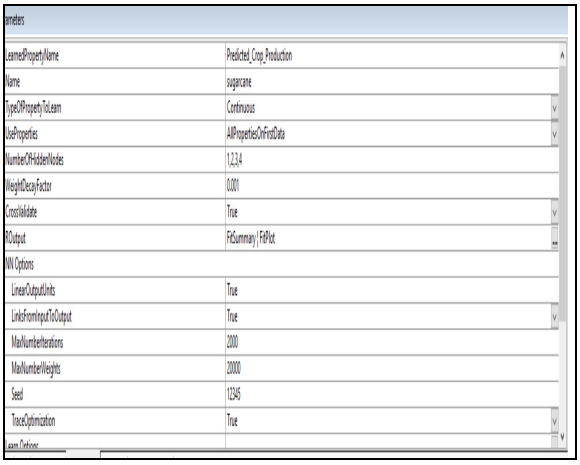


Figure 1.Parameters for the "Learn R Deep Neural Net Model" component

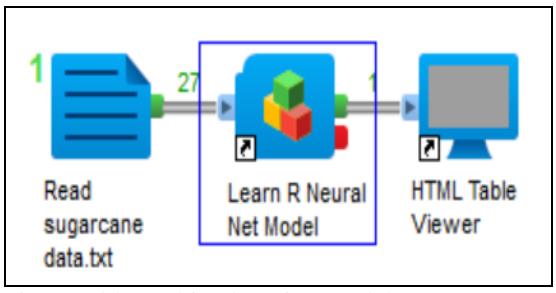


Figure 2 (a) Machine learning model

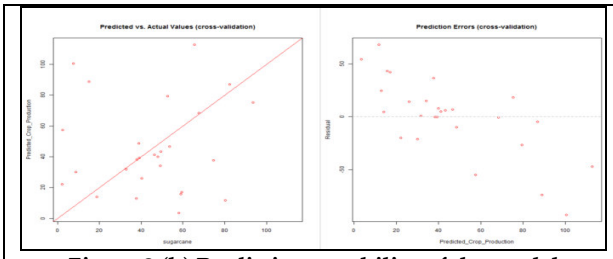


Figure 2 (b) Prediction capability of the model

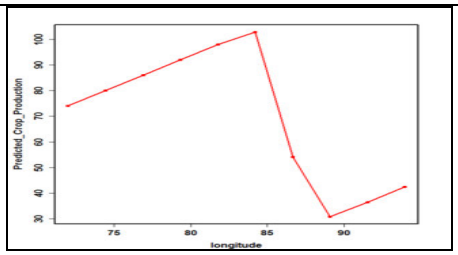
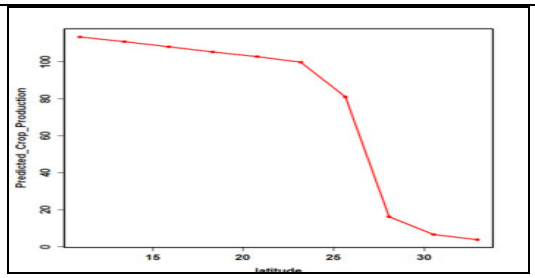


Figure 3: Effect of longitude



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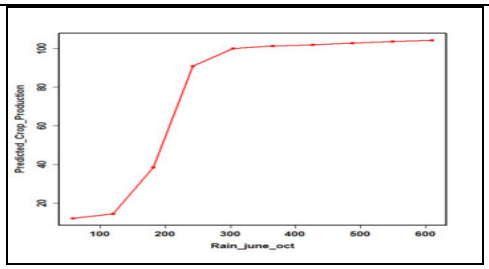

Figure 5: Effect of Rain in Jun-Oct

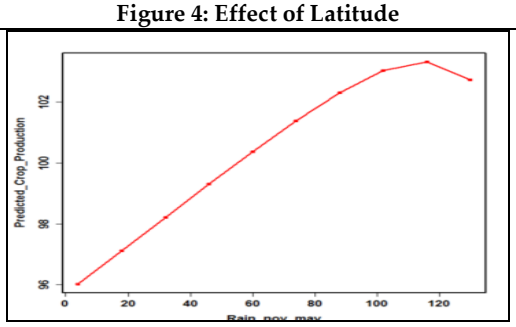

Figure 6: Effect of Rain in Nov-May

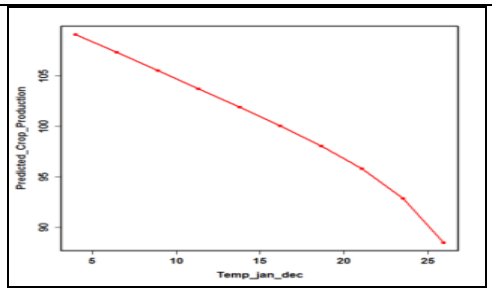

Figure 7: Effect of temperature in Jan-Dec

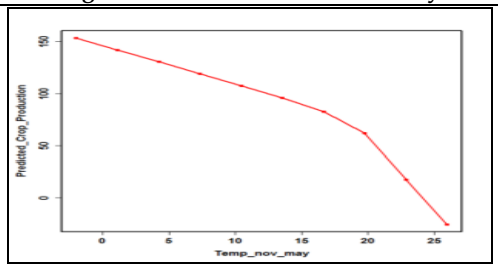

Figure 8: Effect of temp in Nov-May

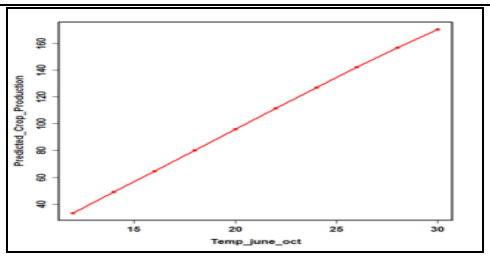

Figure 9: Effect of temp in June-Oct

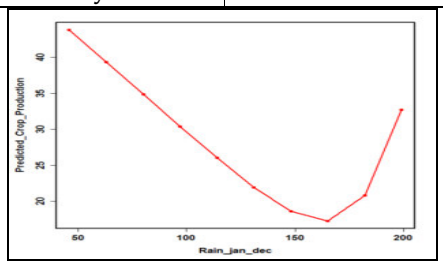

Figure 10: Effect of rain in Jan-Dec

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RESEARCH ARTICLE

Effect of Different Parameters on Production of Wheat Using Machine Learning

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ABSTRACT

Different parameters influence the production of wheat. For the study, the effects of longitude, latitude, Rain and temperature for different seasons on production of wheat was studied. "Pipeline Pilot" module of "Biovia software" (Dassault Systemes of France) was used for analysis. The software provides different built-in components to develop a machine learning model and use the model for prediction.

Keywords: Neural network, Wheat, Latitude, Longitude, Rain, Temperature

INTRODUCTION

Machine Learning

"Machine learning" is an application of "Artificial Intelligence" (AI) that provides systems the ability to automatically learn and improve from experience without being explicitly programmed. "Machine Learning" focuses on the development of computer programs that can access data and use it learn for themselves. "BIOVIA Pipeline Pilot Analytics" and "Machine Learning" offers a comprehensive set of learning and data modelling capabilities, statistical filters and clustering components optimized for large real-world data sets. It gives everything from data cleaning and exploration, to model building, validation, deployment, optimization, and design of future experiments all in a single platform.

Machine learning in agriculture

"Machine learning" is a trending technology nowadays and it can be used in modern agriculture industry. The use of machine learning in agriculture helps to create more healthy seeds. By machine learning agriculture become smarter the applications like

i. Yield prediction and quality assessment
ii. Species identification
iii. Crop disease and weed detection

iv. Diary and egg production
v. Water and soil management etc

Combined with Sensing and Imaging technology "Machine Learning" will be a great boon for agriculture. Via sensors se can sense moisture, humidity, etc. Imaging can give real images of land. Then "machine learning" can assess the conditions for sowing, provide insights on right crop timing, etc. to overall improve productivity. Same way machine learning on land images can help in predicting agriculture related yields / crops etc.
In short machine learning in agriculture is used for smart farming for sustainable agriculture.

Wheat production

"Wheat is the main cereal crop in India. The production of wheat in the country has increased significantly from 75.81 million MT in 2006-07 to an all-time record high of 94.88 million MT in 2011-12. Wheat is the major staple food crop, providing almost half of all calories in the region of North Africa and West and Central Asia. Being next to rice, wheat constitutes one of the key sources of protein in least developed countries and middle-income nations and in terms of calories and dietary intake".

REVIEW OF LITERATURE

"Wheat plays a vital role in the food production as it fulfils 60% requirements of calories and proteins to the 35% of the world population. Owing to wheat importance in food, wheat demand is increasing continuously. Wheat yield is committed to the availability of water supply. Due to climatic and environment variations of different countries, water supply is not available in constant and desire quantity that is necessary for better wheat yield. So, there is a strong relationship and dependency that exists between water supply and wheat yield. Therefore, water supply is becoming an issue because it directly affects wheat yield". In this research, a model is proposed using "Machine Learning" technique to measure the effect of rain, temperature, latitude, longitude on wheat production. Many researchers have done their research work in the area of ML in agriculture. Few of them are listed below:

Cannell et al [1] studied "Effects of waterlogging at different stages of development on the growth and yield of winter wheat". Fortin et al [2] carried out a research study on "A neural network experiment on the site-specific simulation of potato tuber growth in Eastern Canada". Ayoubi and Sahrawat [3] have done a study on "Comparing multivariate regression and artificial neural network to predict barley production from soil characteristics in northern Iran". Pantazi et al [4] investigated "Wheat yield prediction using machine learning and advanced Sensing techniques". Chlingaryan et al [5] done a review on "Machine learning approaches for crop yield prediction and nitrogen status estimation in precision agriculture: A review".Priyanka et al [6] investigated "Agricultural Crop Yield Prediction Using Artificial Intelligence and Satellite Imagery". Recently, Kusum Lata, and Bhushan Chaudhari [7], done a research study on "Crop Yield Prediction Using Data Mining Techniques and Machine Learning Models for Decision Support System".

Objectives

Objective of the present study is to determine the effect of various parameters on production of wheat using machine learning. In this study we can determine the suitable condition where the wheat grows in a manner that we can get maximum profit.

MATERIALS AND METHODS

Software used

"Pipeline Pilot module of Biovia software" (DassaultSystems of France) is used for analysis. The software provides different built-in components to develop a "machine learning model" and use the model for prediction.

Methodology

Collection of data

Data was collected from different sources.Longitude, Latitude, Rainfall, Temperature in different seasons were taken as input while production of wheat was used as output parameter.

Development of deep learning neural network model

The dataset was read using "Delimited Text Reader" component of pipeline pilot. The component was connected to the "Learn R Deep Neural Net Model" component. The output of the model was displayed using "HTML Table Viewer" component. The parameters for the "Learn R Deep Neural Net Model" component were set as shown in Figure 1. The setting for which the experimental output parameter and the predicted parameter were close to a 45^0 line were considered for the final model.

Study of effect of different input parameters on rice production

Text files were prepared where one parameter was varied within the range of data analysed. All other parameters were kept constant at an average value

RESULTS AND DISCUSSION

Wheat production varies due to different reasons. However, the relationships are difficult to predict. Thus, this study focuses on the effect of various input parameters on the wheat production.

Prediction ability of the model

Figure 2(a) shows the model developed.Figure 2(b) shows that the prediction ability of the model was good and the predictions were close to the experimental values.

Prediction by the model

Figure 3 shows that the wheat production in the particular area is gradually decreasing till longitude 80^o E , while the production of wheat is increasing slowly with the increase in longitude above 80^oE. The result shows that low value of longitude favoured wheat production. Figure 4 shows that the production of wheat is gradually increasing if the latitude exceeds 10^o N while the production is decreasing if the latitude above 25^o N. The analysis shows that wheat production is high at around 25^o N. Figure 5 indicates that the production of wheat is gradually decreasing when the rain amount in the month June-October exceeds 100mm. The production of crop is maximum when the rain is less then 100mm. The production of wheat is very high if the rainfall during June-October is low (i.e. 100 mm). Figure 6 shows that the wheat production is gradually increasing in the month November-May when the rain amount is in between 0 mm to 100 mm. And the wheat production is decreasing as the rain amount above 100 mm. Figure 7 represents that the production of wheat is inversely proportional to the temperature in the month January-December. But the temperature between 5^oC to 10^oC, it starts decreasing slowly. Figure 8 shows that the production of wheat is gradually increasing when the temperature is increasing in November-May and after the temperature exceeds 10 the production rate is decreasing continuously. Figure 9 indicates that the production of wheat is inversely proportional to the temperature in June-October i.e. the wheat production is gradually decreasing when the temperature is increasing in June-October. But temperature above 25 production decreasing rate is more. Figure 10 shows that the production of wheat is gradually decreasing if the rain is increasing in between January-December. The production of wheat is maximum when the amount of the rain is minimum in January-December.

CONCLUSIONS

The effects of different parameters on wheat production have been studied using Pipeline pilot. The results shows that wheat production is high at low values of longitude, latitude between 20°N to 25°N and low rainfall(100mm or less) , low temperature areas.

REFERENCES

1. Cannell, R.Q., Belford, R.K., Gales, K., Dennis, C.W., Prew, R.D., 1980. Effects of waterlogging at different stages of development on the growth and yield of winter wheat. J. Sci. Food Agric. 31 (2), 117–132.
2. Jérôme G. Fortin, François Anctil, Léon-Étienne Parent, and Martin A. Bolinder, 2010, "A neural network experiment on the site-specific simulation of potato tuber growth in Eastern Canada", Computers and Electronics in Agriculture, Volume 73, Issue 2, Pages 126-132.
3. Shamsollah Ayoubi and Kanwar Lal Sahrawat (2011): "Comparing multivariate regression and artificial neural network to predict barley production from soil characteristics in northern Iran", Archives of Agronomy and Soil Science, 57:5, 549-565.
4. X.E. Pantazi, D. Moshou, T. Alexandridis, R.L. Whetton, and A.M. Mouazen, "Wheat yield prediction using machine learning and advanced Sensing techniques", Computers and Electronics in Agriculture, 121 (2016), 57 – 65.
5. Anna Chlingaryan, Salah Sukkarieh, and Brett Whelan, "Machine learning approaches for crop yield prediction and nitrogen status estimation in precision agriculture: A review", Computers and Electronics in Agriculture, Volume 151, August 2018, Pages 61-69
6. Teresa Priyanka, Pratishtha Soni, and C. Malathy, "Agricultural Crop Yield Prediction Using Artificial Intelligence and Satellite Imagery", Eurasian J Anal Chem, 2018; 13 (Engineering and Science SP)
7. Kusum Lata, and Bhushan Chaudhari, "Crop Yield Prediction Using Data Mining Techniques And Machine Learning Models For Decision Support System", JETIR, April 2019, Volume 6, Issue 4.
8. Siddique, M. and Panda, D. (2019) Prediction of Stock Index of Tata Steel using Hybrid Machine Learning Based Optimization Techniques, International Journal of Recent Technology and Engineering, Vol. 8 (2): 3186-3193.
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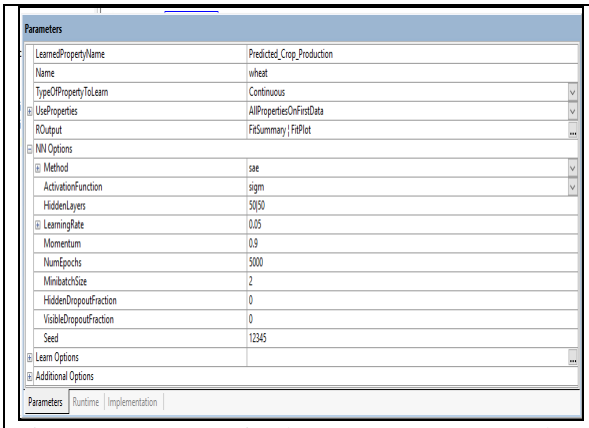

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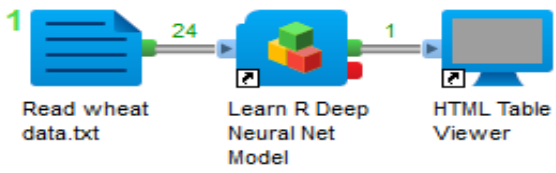

Figure 2(a) Machine learning model

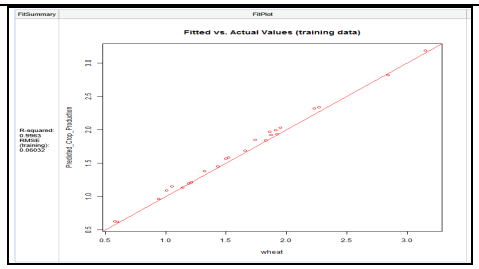

Figure 2 (b) Prediction capability of the model

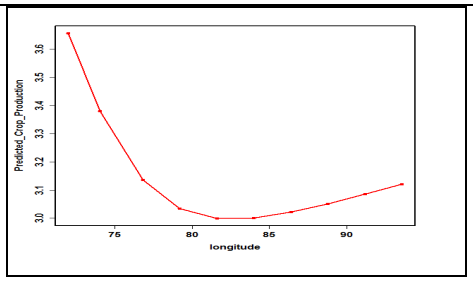

Figure 3: Effect of longitude

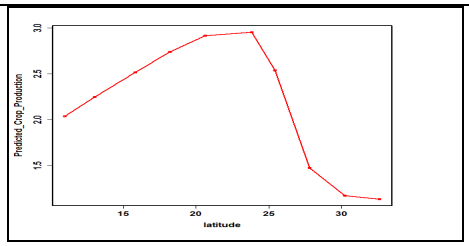

Figure 4: Effect of Latitude

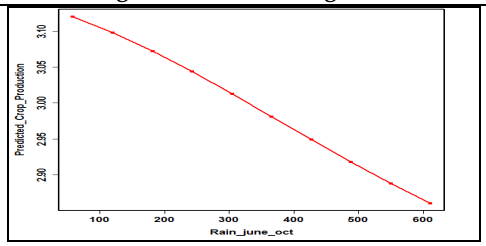

Figure 5: Effect of Rain in Jun-Oct

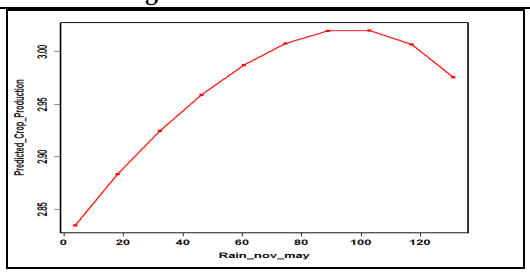

Figure 6: Effect of Rain in Nov-May

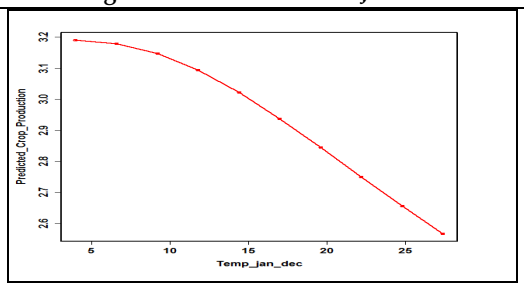

Figure 7: Effect of temperature in Jan-Dec

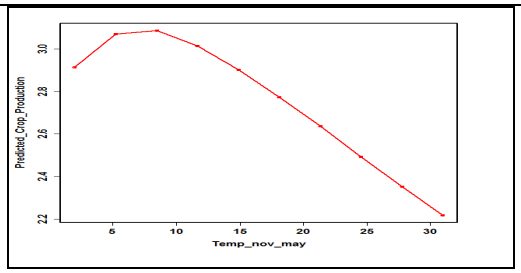

Figure 8: Effect of temp in Nov-May

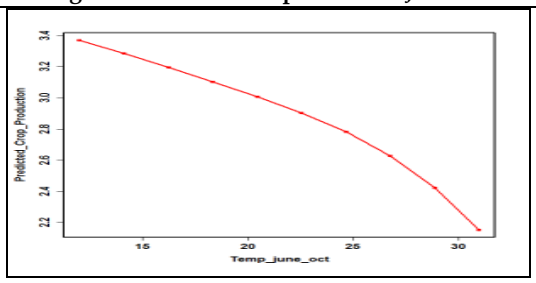

Figure 9: Effect of temp in June-Oct

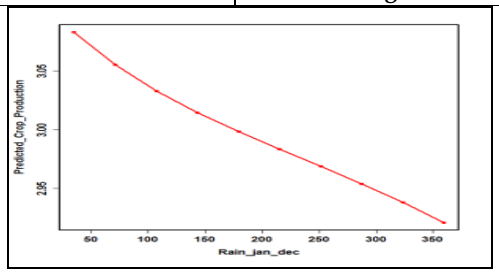

Figure 10: Effect of rain in Jan-Dec

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RESEARCH ARTICLE

On the Oscillation and Non-Oscillation of Class of Second Order Difference Equations

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ABSTRACT

In this article we obtain some sufficient conditions in term of coefficients for the oscillation and nonoscillation of solutions of following difference equation $\Delta_\alpha\left(s_m\Delta_\alpha x_m\right)+t_m\Delta_\alpha x_m=G\left(m,x_m,\Delta_\alpha x_m\right)$. Where, $m\geq 0$ and $\alpha>0$.

Keywords: Generalized difference equation, oscillatory and non-oscillatory behaviour.

INTRODUCTION

The theory of difference equation is significant for its wide range of applications in numerical analysis, control theory, finite mathematics, statistics, economics, biology and Computer Science etc. For example, if a certain population has discrete generations, the size of $\left(\mathrm{k}+1\right)^{\mathrm{th}}$ generation y_{k+1} is a function of the k^{th} generation y_k. The relation expresses itself in the difference equation $y_{k+1}=f(y_k)$. An equation of the form $f(k,z_k,\Delta z_k,\Delta^2 z_k.....)=0$ is called difference equation. Where, Δ is the forward difference operator. And the forward difference operator defined as $\Delta z_k=z_{k+1}-z_k$. Though non-linear difference equations are little bit difficult to analyse than linear difference equations. Some linear representations do not get sufficiently accurate model for physical systems. Thus the study of nonlinear difference equations is both an interesting and useful area of research. So there is a need to study oscillatory and non-oscillatory theory of difference equations. For the basic theory of difference equations and its application, one can refer the monograph of Agarwal [8], Kelly & Peterson [10] and Lakshmikanthan and Trigiante [9]. For the past few decades, there has been a lot of interest in the study of oscillatory behavior of solutions of difference equations. For example, E. Thandapani; K. Mahalingam [3], S.S. Cheng

and W. Patula [7], B. G. Zhang and Y. Zhou [1], N.Parhi [6] have done extensive work on this topic. J. Popenda [4] discussed the oscillatory and non-oscillatory behaviour of the solutions of some second-order difference equations in the from $\Delta_a^2 x_n = f(n, x_n, \Delta_b x_n)$. B. Szmanda [2] gives the idea about non oscillation, oscillation growth of the solutions of the nonlinear difference equation of second order in the form $\Delta(r_n \Delta u_n) + a_n f(n, u_n, \Delta u_n) = g(n, u_n, \Delta u_n)$.

Here we obtained sufficient conditions for oscillatory and nonoscillatory behaviour of solutions of following generalized difference equation.

$$\Delta_\alpha \left(s_m \Delta_\alpha x_m\right) + t_m \Delta_\alpha x_m = G\left(m, x_m, \Delta_\alpha x_m\right) \qquad (1)$$

Where, $m \geq 0$ and $\{s_m\}, \{t_m\}$ are real sequences such that $s_m > 0$ for $m \geq n$. The generalized difference operator Δ_a for $a \neq 0$, is defined as $\Delta_a z_n = z_{n+1} - a z_n$ and $G : N \times R^2 \to R$, $X : N \to R$. Here we denote $\{x_m\}$ as the class of non-trivial solutions of (1) i.e. a solution of difference equations (1) and for every, $i \in N, \exists n > i$ such that $x_n \neq 0$ and $X_1 = \{x_m \in X : \Delta_\alpha x_k = 0 \text{ holds for } k \in N\}$, $X_2 = X - X_1$.

The corresponding homogeneous difference equation can be written as

$$\Delta_\alpha \left(s_m \Delta_\alpha x_m\right) + t_m \Delta_\alpha x_m = 0. \qquad (2)$$

Oscillatory solution of equation (1) we mean it is neither eventually positive nor eventually negative. Else it is termed as nonoscillatory solution .

Oscillatory Behaviour

In this section we studied oscillatory and non-oscillatory behaviour of equation (1) and (2).

Lemma 2.1

[5] Let $\{x_m\}$ be a real sequence. If $\{\Delta_\alpha x_m\}, \alpha > 0$, is eventually of one sign, then $\{x_m\}$ is eventually of one sign.

Lemma 2.2

[5] For $\alpha > 0$, a real sequence $\{x_m\}$ is oscillatory if $\{\Delta_\alpha x_m\}$ is oscillatory.

Proposition 2.3

If $s_m \leq t_m$ then all solutions of equation (2) are oscillatory.

Proof: From equation (2) we obtain

$$\Delta_\alpha x_{m+1} = \frac{1}{s_{m+1}}\left[\left(s_m - t_m\right)\Delta_\alpha x_m\right] \qquad Or$$

$$\Delta_\alpha x_m \Delta_\alpha x_{m+1} = \frac{1}{s_{m+1}}\left[\left(s_m - t_m\right)\left(\Delta_\alpha x_m\right)^2\right] \leq 0$$

$\Rightarrow \Delta_\alpha x_m$ and $\Delta_\alpha x_{m+1}$ are of opposite sign.

Repeating the above procedure we obtain $\Delta_\alpha x_m$ is oscillatory that implies $\{x_m\}$ is oscillatory.

Proposition 2.4

If $s_m > t_m$ then all solutions of equation (2) are non-oscillatory.

Proof of the Proposition 2.4 follows from Proposition 2.3 and lemma 2.1.

Proposition 2.5

For $\alpha > 0$, if the equation (1) and satisfies the condition

$$\begin{cases} G(m,w,z) = 0 \ \ if \ \ z = 0 \\ \dfrac{z}{s_{m+1}}\left[G(m,w,z) + (\alpha s_m - t_m)\, \mathrm{Z} \right] \geq 0, if\ z \neq 0 \end{cases} \qquad (3)$$

For $m \in N$ and $w, z \in R$, then all non-trivial solutions of equation (1) are non-oscillatory.

Proof: Let's choose $\{x_m\}$ be the non-trivial solution of equation (1).

So either $x_m \in X_1 \, or \, x_m \in X_2$

In the 1st case let's choose $x_m \in X_1$

$\Rightarrow \Delta_\alpha x_k = x_{k+1} - \alpha x_k = 0 \ \ \forall k \in N$

So the 1st condition of equation (2) satisfies

$G(m,w,z) = 0$

For $m = \beta$ in equation (1) we get,

$\Delta_\alpha \left(s_\beta \Delta_\alpha x_\beta \right) = 0$

$\Rightarrow s_{\beta+1} \Delta_\alpha x_{\beta+1} - \alpha s_\beta \Delta_\alpha x_\beta = 0$

$\Rightarrow \Delta_\alpha x_{\beta+1} = \dfrac{\alpha s_\beta}{s_{\beta+1}} \Delta_\alpha x_\beta = 0$

Repeating this process we get $\Delta_\alpha x_{\beta+2} = 0$

So by method of induction we can easily derive,

$\Delta_\alpha x_{\beta+i} = 0, i \in N$

So $x_{\beta+i} = \alpha^i x_\beta \quad , i \in N$

$\because \alpha > 0 \, and \, x_\beta \neq 0$

Thus $x_{\beta+i}$ is eventually positive or negative as $x_\beta > 0 \, \text{or} \, x_\beta < 0$

Let us take $x_m \in X_2$ and assumes x_m is oscillatory.

Then either $(a)\ x_\beta > 0 \ , x_{\beta+1} \leq 0$ or $(b) x_\beta \geq 0 \ \ , x_{\beta+1} < 0$ holds for some $\beta \in N$

In both case we have $\Delta_\alpha x_\beta < 0$ (4)

By rewriting equation (1) we get

$$\Delta_\alpha x_{m+1} = \frac{1}{s_{m+1}}\left[G(m, x_m, \Delta_\alpha x_m) + (\alpha s_m - t_m) \Delta_\alpha x_m \right] \qquad (5)$$

Let's take $m = \beta$ in equation (5) and multiplying $\Delta_\alpha x_\beta$ both sides we get

$$\Delta_\alpha x_\beta \Delta_\alpha x_{\beta+1} = \frac{\Delta_\alpha x_\beta}{s_{\beta+1}}\left[G\left(\beta, x_\beta, \Delta_\alpha x_\beta\right)+\left(\alpha s_\beta - t_\beta\right)\Delta_\alpha x_\beta\right]$$

$$\Rightarrow \Delta_\alpha x_\beta \Delta_\alpha x_{\beta+1} \geq 0 \qquad (6)$$

Repeating this process we get, $\Delta_\alpha x_{\beta+i} < 0 \ \forall i \in N$

$\because \alpha > 0 \, and \, x_{\beta+1} \leq 0$

So $x_{\beta+i+2} < \alpha^{i+1} x_{\beta+1} \leq 0$, a contradiction.

Hence x_m is non-oscillatory.

Proposition 2.6

If $\alpha > 0$ and satisfies the condition

$\frac{z+\alpha w}{s_{m+1}}\left[G\left(m,w,z\right)+\left(\alpha s_m + t_m\right)z\right] \geq 0$ for $m \in N$ and $w, z \in R$, where $z + \alpha w \neq 0$, then all non-trivial solution of equation (1) are non-oscillatory.

Proof: Here $z + \alpha w = \Delta_\alpha x_m + \alpha x_m = x_{m+1} - \alpha x_m + \alpha x_m \neq 0$

Let $x_m \in X$ be any non-trivial solution of equation (1) then for some $\beta \in N$, we get $x_{\beta+1} \neq 0$

Let $m = \beta$ in equation (5) and multiplying $x_{\beta+1}$ on both sides we get,

$$x_{\beta+1}\Delta_\alpha \, x_{\beta+1} \geq 0 \qquad (7)$$

a) If $x_{\beta+1} > 0$ then in equation (7) $\Delta_\alpha x_{\beta+1} \geq 0$

And hence $x_{\beta+2} \geq \alpha x_{\beta+1}$ by method of induction we have,

$x_{(\beta+i+1)} \geq \alpha^i x_{(\beta+1)} > 0 \ \forall i \in N$. So x_m is eventually positive solution.

b) If $x_{\beta+1} < 0$, from (7) we get, $\Delta_\alpha x_{\beta+1} \leq 0$. So $x_{\beta+2} \leq \alpha x_{\beta+1} < 0$

By of method induction we have, $x_{\beta+i+1} \leq \alpha^i x_{\beta+1} < 0 \, \forall i \in N$ .So x_m is eventually negative.

Proposition 2.7

If $\alpha < 0$ and satisfies the condition

$$\begin{cases} G\left(m,w,z\right) = 0 \ \ if \ \ z = 0 \\ \frac{z}{s_{m+1}}\left[G\left(m,w,z\right)+\left(\alpha s_m - t_m\right)\mathbf{Z}\right] \geq 0, if \ z \neq 0 \end{cases} \qquad (8)$$

For $m \in N$ and $w, z \in R$, then all non-trivial solutions of equation (1) are oscillatory.

Proof: Let's consider that $\{x_m\}$ be any non-trivial solution equation (1) so it must satisfy either $x_m \in X_1 \, or \, x_m \in X_2$

If $x_m \in X_1$ then $\Delta_\alpha x_k = x_{k+1} - \alpha x_k = 0$ for some $k \in N$ and by condition (1) of (8) we have, $G\left(m,w,z\right) = 0$.

For $m=\beta$ in equation (1) $\Delta_\alpha x_{\beta+1}=\dfrac{\alpha s_\beta}{s_{\beta+1}}\Delta_\alpha x_\beta=0$

By method of induction we get, $\Delta_\alpha x_{\beta+i}=0$

$\Rightarrow x_{\beta+i}=\alpha^i x_\beta$ holds for some $i\in N$

So we have $x_{\beta+i}x_{\beta+i+1}=\alpha^{2i+1}x_\beta^2<0$.Hence x_m is oscillatory.

If $x_m\in X_2$, by 2nd condition of equation (8) we have

$$\frac{\Delta_\alpha x_m}{s_{m+1}}\left[G(m,w,z)+(\alpha s_m-t_m)\Delta_\alpha x_m\right]\le 0$$

Let us assume the contrary i.e x_m is non-oscillatory.

Then it must be either eventually positive or eventually negative.

If $x_m>0$ for $m\ge\beta$, where β is an even integer.

Let $m=\beta$ in equation (4) and multiplying $\Delta_\alpha x_\beta$ both sides we get,

$$\Delta_\alpha x_\beta\Delta_\alpha x_{\beta+1}\le 0$$

$$\Rightarrow\left(x_{\beta+1}-\alpha x_\beta\right)\left(x_{\beta+2}-\alpha x_{\beta+1}\right)\le 0$$

$$\Rightarrow\alpha^{\beta+1}\left(\frac{x_{\beta+1}}{\alpha^{\beta+1}}-\frac{x_\beta}{\alpha^\beta}\right)\alpha^{\beta+2}\left(\frac{x_{\beta+2}}{\alpha^{\beta+2}}-\frac{x_{\beta+1}}{\alpha^{\beta+1}}\right)\le 0$$

$$\Rightarrow\alpha^{\beta+1}\alpha^{\beta+2}\left[\Delta\left(\frac{x_\beta}{\alpha^\beta}\right)\Delta\left(\frac{x_{\beta+1}}{\alpha^{\beta+1}}\right)\right]\le 0$$

$$\Rightarrow\ \Delta\left(\frac{x_\beta}{\alpha^\beta}\right)\Delta\left(\frac{x_{\beta+1}}{\alpha^{\beta+1}}\right)\ge 0 \qquad (9)$$

$\because\alpha<0$ and $\Delta_\alpha x_\beta=\alpha^{\beta+1}\Delta\left(\dfrac{x_\beta}{\alpha^\beta}\right)$

If $\Delta\left(\dfrac{x_\beta}{\alpha^\beta}\right)\ge 0$ then $\dfrac{x_{\beta+1}}{\alpha^{\beta+1}}\ge\dfrac{x_\beta}{\alpha^\beta}>0$ holds

We get $x_{\beta+1}<0$ which is contradiction that $x_m>0$ holds for $m\ge\beta$

Again if $\Delta\left(\dfrac{x_\beta}{\alpha^\beta}\right)<0$

$$\Rightarrow\Delta\left(\frac{x_{\beta+1}}{\alpha^{\beta+1}}\right)\le 0$$

i.e $\dfrac{x_{\beta+2}}{\alpha^{\beta+2}}\le\dfrac{x_{\beta+1}}{\alpha^{\beta+1}}$

$\because \alpha < 0, x_{\beta+1} > 0$ and $\beta \in N$ is an even integer so $\frac{x_{\beta+2}}{\alpha^{\beta+2}} < 0$

Therefore $x_{\beta+2} < 0$ ($\because \beta$ is even integer).

Similarly we can prove for $x_m < 0$.

Proposition 2.8

If $\alpha < 0$ and satisfies the condition

$$\frac{z+\alpha w}{s_m+1}\left[G\left(m, x_m, \Delta_\alpha x_m\right)+\left(\alpha s_m + t_m\right)z\right] \le 0 \qquad (10)$$

For $m \in N$ and $w, z \in R$, $z + \alpha w \neq 0$ then all non-trivial solution of equation (1) are oscillatory.

Proof: Here $z+\alpha w = \Delta_\alpha x_m + \alpha x_m = x_{m+1} - \alpha x_m + \alpha x_m \neq 0$

From equation (10) we get,

$$\frac{x_{m+1}}{s_m+1}\left[G\left(m, x_m, \Delta_\alpha x_m\right)+\left(\alpha s_m + t_m\right)z\right] \le 0 \text{ For } x_{m+1} \neq 0 \qquad (11)$$

Let $x_m \in X$ be any non-trivial solution of equation (1) then there is $\beta \in N$ such that $x_{\beta+1} \neq 0$

Let $m = \beta$ in equation (5) and multiplying $x_{\beta+1}$ both sides we get,

$$x_{\beta+1}\Delta_\alpha x_{\beta+1} \le 0 \qquad (12)$$

i) If $x_{\beta+1} > 0$ then by equation (12) we have $\Delta_\alpha x_{\beta+1} \le 0$

Hence $x_{\beta+2} \le \alpha x_{\beta+1} < 0$

ii) If $x_{\beta+1} < 0$ then by equation (12) we have $\Delta_\alpha x_{\beta+1} \ge 0$ and hence

$x_{\beta+2} \ge \alpha x_{\beta+1} > 0$

Proceeding as above we get, $x_{\beta+i}x_{\beta+i+1} < 0$ is true for $i \in N$ .So $\{x_m\}$ is oscillatory.

By putting $s_m = 1$ and $t_m = 0$ for $m \in N$ equation (1) reduces to

$$\Delta_\alpha^2 x_m = G\left(m, x_m, \Delta_\alpha x_m\right) \quad m \in N \qquad (13)$$

Corollary 2.9

If $\alpha > 0$ and satisfies the condition $\begin{cases} G\left(m, x_m, \Delta_\alpha x_m\right) = 0 \text{ if } \Delta_\alpha x_m = 0 \\ \Delta_\alpha x_m\left[G\left(m, x_m, \Delta_\alpha x_m\right)+\alpha\Delta_\alpha x_m\right] \ge 0 \text{ if } \Delta_\alpha x_m \neq 0 \end{cases}$ (14)

Where $m \in N$ and $w, z \in R$

Then all non-trivial solutions of (13) are non-oscillatory

Proof of the corollary 2.9 follows from Proposition 2.5.

Corollary 2.10

If $\alpha > 0$ and satisfies the condition

For $m \in N$ and $w, z \in R$ with $z + w\alpha \neq 0$

$$(z+w\alpha)[G(m,x_m,\Delta_\alpha x_m)+\alpha(z)]\geq 0 \quad (15)$$

Then all non-trivial solutions of (13) are non-oscillatory

Proof of the corollary 2.10 to 2.11 follows from Proposition 2.6.

Corollary 2.11: If $\alpha<0$ and satisfies condition

$$\begin{cases} G(m,x_m,\Delta_\alpha x_m)=0 \text{ if } \Delta_\alpha x_m=0 \\ \Delta_\alpha x_m\left[G(m,x_m,\Delta_\alpha x_m)+\alpha\Delta_\alpha x_m\right]\leq 0 \text{ if } \Delta_\alpha x_m\neq 0 \end{cases} \quad (16)$$

Where $m\in N$ and $w,z\in R$

Then all non-trivial solutions of equation (13) are oscillatory.

Proof of the corollary 2.10 follows from Proposition 2.7

Corollary 2.12

If $\alpha<0$ and satisfies condition

For $m\in N$ and $w,z\in R$ with $z+w\alpha\neq 0$

$$(z+w\alpha)[G(m,x_m,\Delta_\alpha x_m)+\alpha(z)]\geq 0 \quad (17)$$

Then all non-trivial solutions of equation (13) are oscillatory

Proof of the corollary 2.11to 2.12 follows from Proposition 2.8.

CONCLUSION

We obtained some sufficient conditions for oscillatory and non-oscillatory behavior of solutions of non-linear difference equations. Further we can also study the asymptotic behavior and stability of non-liner difference equation. Also higher order non-linear difference equations can be considered to analysis the qualitative behavior of solutions of difference equation.

REFERENCES

1. B. G. Zhang and Y. Zhou, "Oscillation and Non oscillation of Second Order Linear Difference Equations", J. Comp. & Math with Appl., Vol.39, 1-7, 2000.
2. B. Samanda, Nonoscillation, "Oscillation and growth of solutions of nonlinear difference equations of second order", J. Math. Anal. Appl. 109, 22-30, 1985.
3. E. Thandapani; K. Mahalingam, "Oscillation and nonoscillation of second order neutral delay difference equations", Czech. Math. Journal. Vol. 53, No. 4, 935–947, 2003.
4. J. Popenda, Oscillation and nonoscillation theorems for second-order difference equations, J. Math. Anal.Appl. 123, 34-38, (1987).
5. N.Parhi, Anita Panda, "Non oscillation and oscillation of solution of class of third order difference equations", J. Math. Anal. Appl. 336, (2007) 213-223.
6. N. Parhi, "Oscillation and non-oscillation of solutions of second order difference equations involving generalized difference", Appl. Math. and Comp, Vol. 218, 458-468, 2011.
7. S.S. Cheng, and W. Patula, "An Existence Theorem for a Nonlinear Difference Equations", Nonlinear Anal.20, (1992), 193-2013.
8. R.P. Agarwal, "Difference equations and inequalities", Marcel Dekker, 2nd edition, New York, 2000.
9. V. Lakshmikantham and D. Trigiante, "Theory of Difference Equations: Numerical Methods and Applications", Academic Press, New York, 1988S.
10. W.G. Kelly and A.C. Peterson, "Difference Equations: An Introduction with Applications", Academic Press, New York, 1991.

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RESEARCH ARTICLE

Maintenance Allocation Model of Wire EDM by using Fuzzy Logic

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ABSTRACT

The paper's goal is to build a computer based, proactive maintenance scheduling and fault diagnosis model for CNC wire EDM that reduces the mean repair time and provides a timely optimization for a given model. The model established plays significant processes in predicting and diagnosing of WEDM faults on site through expert guidance to support CNC. This paper suggested a questionable rule- based model for Wire – EDM's maintenance schedule and fault-diagnosis. This method is a powerful development tool for a complicated consulting method like a Wire EDM project, thanks to the advantages of fuzzy logic. The design software will accompany with trainer and fabrication worker by explaining the fault diagnosis and fault therapy. Through easily detecting faults it can help achieve trouble- free and smooth machining. A simulation model for predict the maintenance requirement of machine components operating under established conditions will be built.

Keywords: Wire EDM, Fuzzy logic and Simulation model

INTRODUCTION

Maintenance Item Allocation Model is a constructive maintenance scheduling model based on the computer, which decreases the mean repair time. Maintenance obligation predicated on real or imminent failure preferably maintenance is done to maintain equipment and system working effectively for the component's design life at least. Past and existing maintenance procedures in both the private and government sectors will suggest that maintenance is the steps concerned with fixing equipment after it has been broken. This will mean that maintenance steps must be taken to avoid the failure or fixation of from failing normal equipment failure associated with the operation of the system by a computer or part to maintain in the proper working order. Sadly, data

collection in several surveys over the past decade shows that most private and government facilities do not expand the required resources in proper working order to maintain equipment. Instead, they anticipate failure of equipment and then take whatever action is necessary to fix or remove the equipment.Design and testing of the m odel will be focused on knowledge and statistics of the current operations and maintenance activities.This saves time in the acquisition of knowledge, is easy to manage and can self-learn. Suggestions to remove faults are introduced sequentially according to the priority assumed once a fault occurs.

Wire EDM

Wire electrical discharge machining (WEDM) is a commonly recognized method for the removal of nontraditional m aterials used to create components with complex shapes and profiles.It is considered a novel modification of the mod ern EDM process, which initializes the sparking cycle using an electrode. WEDM, however, uses a continuously moving wire electrode made of thin 0.05-0.3 mm diameter copper, brass or tungsten, which can achieve very low corner radii. Using a mechanical tensioning tool, the wire is held in tension which reduces the propensity to produce inaccurate parts. The material is eroded in front of the wire during the WEDM process and there is no direct interaction between work piece and the wire, thereby reducing the mechanical stresses during machining. Furthermore, the WEDM process is capable of machining exotic and high strength and temperature resistive (HSTR) materials and removing the geometric changes that occur in the production of heat-treated steels. It was introduced in the late 1960s', and has revolutionized the tool and die, mold, and metalworking industries. It was only towards the end of the 1970s, when computer numerical control (CNC) system was initiated into WEDM that brought about a major evolution of the machining process. Due to the wire, which has to move through the component to be machined, the WEDM process was extensively used for any by hole machining. WEDM's popular applications include the manufacture of stamping and extrusion tools and dies, fixtures and gages, prototypes, aircraft and medical components, and equipment for the grinding wheel. The manufacturing scenario has changed dramatically in today's metal cutting industry, based on an automated factory model, in view of achieving higher performance through consistent efforts by the manufacturing engineer.

Principle of Wire Electrical Discharge Machining

Typical WEDM configuration consists of cable, running, electrical and electronic control unit, electrical power supply, cable feed drive and dielectric supply system. WEDM's material removal mechanism is very similar to traditional EDM process involving the erosion effect created by electrical (sparks) discharges. In WEDM, material is eroded from the work piece by a series of distinct sparks that occurs between the piece of work and the wire separated by a stream of dielectric fluid that is continuously fed into the machining field. The CNC machine performs functions such as serial cutting operation, partial modeling and generation of CNC code, wire feed, working motion, dielectric The CNC machine performs functions such as serial cutting operation, partial modeling and generation of CNC code, wire feed, working motion, dielectric circulation, wire diameter comp ensation, etc. Owing to its superior reaction time (approx. 2μs), the electro hydraulic servo control system is generally over the electromechanical servo system.

The key benefit of a servo control system is that it allows the device to withdraw in the event of a short circuit around the gap before the right distance (ranging from 0.025 to 0.05 mm) is calculated. The work piece is clamped on the worktable (X-Y). The table is driven by D.C servo motors along X and Y-axis directions. Continuously fed from a wire supply spool, the wire electrode passes through the wire guide where it selects the necessary current cutting the work piece under defined tension. The used wire is directed to a chopper. The chopped pieces are collected in a collection bin. The upper wire guide supported to the auxiliary table (U-V) can be moved along U and V-axis with respect to the stationary lower wire guide. By moving the quill, the upper wire guide can also be vertically positioned along Z-axis to accommodate various job thicknesses. The path information of X-Y table and U-V table is passed to the controller in terms of linear and circular interpolations via NC program. A series of electrical pulses generated by the pulse generator unit is applied between the work piece and the travelling wire electrode, to cause

the electro erosion of the work piece material. As the process proceeds, the X-Y controller moves the worktable carrying the work piece transversely along a predetermined path programmed in the controller. While machining is in progress, the machining zone is continuously flushed with distilled water (dielectric medium) passing through the nozzle on both sides of the work piece.

Problem Formulation

It is quiet complicated and expensive machine and only few units of EDM are found in an industry. It is a time consuming process and some faults such as wire breaking, dielectric losing its strength exaggerated the total processing time. Although it is a good technique for industrial application but still there are some problems associated with it. In order to overcome such problem a fuzzy rule based model and bond graph model is developed to avoid wire breakage and to diagnose the fault in dielectric system respectively, which helps in quick detection of fault and hence improves maintenance efficiency.

Fuzzy Logic

Fuzzy logic, originally developed by LoftiZadeh, Professor of the University of California at Berkeley, is an attempt to model human experience and intuition. Zadeh stated that the rigidity of conventional set theory made it impossible to properly account for the vagueness that is commonplace in the real world. In conventional set theory, elements are either a member of a given set or they are not. There is no middle ground. In fuzzy set theory, an element's membership in a set is a matter of degree. An element may also be a member of more than one set. A common way of applying fuzzy sets is to represent human knowledge or rules of thumb in the form of IF-THEN logical statements, also known as rules. In a fuzzy logic system only the elements being manipulated are fuzzy; the rules of logic are well defined. The opposite concept to fuzzy is crisp. The crisp world is a binary world that can be represented by yes and no, 0 and 1. A lot of applications can be processed with crisp logic. But fields such as expert systems, decision making, pattern recognition, product design, and machine monitoring require more than crisp logic. Membership functions span some problem domain and show the degree of membership of each value in the problem domain in that function. Membership functions are subjective evaluations and can be in any kinds of curve. Membership functions, however, cannot be assigned arbitrarily. A fuzzy variable would then consist of degrees of membership in these membership functions for a given output.

Fuzzy Knowledge Base

Figure 3 shows the triangle-shaped membership functions of input variables
VL - very low value (range is -1.25 to 3)
L - Low value (range is 1 to 5)
M - Medium value (range is 3 to 7)
H - High value (range is 5 to 9)
VH - very high value (range is 7 to 11)

The Mamdani algorithm is the inference technique used in this framework. The fuzzy sets are designated by the labels:
VL - very low value (range is -1.25 to 2)
L - low value (range is 1 to 4)
M - medium value (range is 3 to 7)
H - high value (range is 6 to 9)
VH - very high value (range is 8 to 11)

Design a Fuzzy Rules

The design of a fuzzy system, the first step refers to the collection of the available information. It has two have two forms: human experience and sampled input-output pairs recorded by the human expert. Human experience is presented as a set of IF-THEN rules explaining under what conditions what action should be taken. The sampled pairs give numerical information concerning the inputs and the outputs. This consisted of the generation of fuzzy rules from numerical data pairs, the collection of the fuzzy rules into a common FAM, and finally, designing a control system based on the FAM bank using the centroid defuzzifying method.

Membership Functions

To associate crisp inputs with fuzzy sets, you need to identify membership functions. The triangular membership functions are used for computational efficiency for variable inputs and outputs. The three fuzzy sets (wire tension, wear & tear at wire guide and inter electrode gap) are proposed for the inputs and one (wire breakage) for the output (Fig. 5). The membership functions for input fuzzy sets are selected as follows: 1 as very low value (VL), 2 as low value (L), 3 as medium value (M), 4 as high value (H) and 5 as very high value (VH). Similarly the output fuzzy sets are defined in this order: 1 as very low value (VL), 2 as low value (L), 3 as medium value (M), 4 as high value (H) and 5 as very high value (VH).

Rule no- 23: IF wire tension is very low, wear & tear at wire guide is very high , inter electrode gap is medium THEN wire breakage is medium.
Rule no- 45 : IF wire tension is low, wear & tear at wire guide is high , inter electrode gap is very high THEN wire breakage is high.
Rule no-82 : IF wire tension is high, wear & tear at wire guide is low , inter electrode gap is low THEN wire breakage is medium.
Rule no- 102: IF wire tension is high, wear & tear at wire guide is very low , inter electrode gap is low THEN wire breakage is low.

RESULT AND DISCUSSION

A fuzzy model for the maintenance-schedule and fault-diagnosis of wire EDM is developed. It is time-saving in knowledge acquisition, is easy to maintain and is capable of self-learning. The role of this fuzzy inference engine is to perform the fuzzy operations necessary for the determination of the fault cause. The model works according to the fuzzy inputs and the activated rules and provides a very quick response.
Description for input and output variables along with their membership function and range are given as follows:

[Input1]
Name=']_wire tension'
Range=[1 10]
NumMFs=5
MF1='very_low':'trimf',[-1.25 1 3]
MF2='low':'trimf',[1 3 5]
MF3='medium':'trimf',[3 5 7]
MF4='high':'trimf',[5 7 9]
MF5='very_high':'trimf',[7 9 11]
[Input2]
Name='wear_&_tear_at_wire_guide'
Range=[1 10]
NumMFs=5
MF1='very_low':'trimf',[-1.25 1 3]

MF2='low':'trimf',[1 3 5]
MF3='medium':'trimf',[3 5 7]
MF4='high':'trimf',[5 7 9]
MF5='very_high':'trimf',[7 9 11]
[Input3]
Name='inter electrode gap'
Range=[1 10]
NumMFs=5
MF1='very_low':'trimf',[-1.25 1 3]
MF2='low':'trimf',[1 3 5]
MF3='medium':'trimf',[3 5 7]
MF4='high':'trimf',[5 7 9]
MF5='very_high':'trimf',[7 9 11]
[Output1]
Name='wire breakage'
Range=[1 10]
NumMFs=5
MF1='very_low':'trimf',[-1.25 1 2]
MF2='low':'trimf',[1 2.5 4]
MF3='medium':'trimf',[3 5 7]
MF4='high':'trimf',[6 7.5 9]
MF5='very_high':'trimf',[8 9.5 11]

CONCLUSIONS

The following conclusions are drawn on the basis of an established Fuzzy rule based model for WEDM fault diagnos is and maintenance:

1) Based on this, minimization of wire breakage and maintaining the machining accuracy due to input parameters will be made.
2) Wastage of wire can be minimized by reducing the feed rate depending on input parameters. This will help in reducing the down time and increase productivity.
3) The developed model can meet the requirement of the manufacturing industry through fault findings on WEDM in a short cycle of time and enhance the productivity by reducing the lead time.
4) This designed method can also be applied to other fault diagnostic applications, where the input and output module are specific and well defined.

REFERENCES

1. Snoeys. R and Dekeyser. W (1988), Knowledge- Based System for Wire-EDM, "The International Journal of Advanced Manufacturing Technology", vpl-3, 83-96.
2. KadarsahSuryadi, Eri Ricardo Nurzal (1998), A Decision Support System for Car Fault Diagnosis Using Expert System. "International Journal of Information Sciences for Decision Making", Page 75-78.
3. Makis. V, Jiang. X, and Jardine A. K. S. (1998), A condition based maintenance model , "IMA Journal of Mathematics Applied in Business & Industry" ,vol-9, 201-210.
4. Celso Marcelo F. Lapaa, Claudio Marcio N.A. Pereira ,MarcioPaes de Barros (2006), A model for preventive maintenance planning by genetic algorithms based in cost and reliability, "Reliability Engineering and System Safety", vol-91 ,233–240.

5. Thomas R. Pomorski (2004), Total Productive Maintenance (TPM) Concepts and Literature Review, "Total Productive Maintenance Concepts and Literature Review" April 30, 2004.
6. Williams.G.B. (1998) ,An intelligent maintenance model (system):an application of the analytic hierarchy process and a fuzzy logic rule-based controller, "Journal of the Operational Research Society" vol-49, 745-757.
7. Liu. T. I. (1996), detection of roller bearing defects using expert system and fuzzy logic, "Mechanical Systems and Signal Processing" vol-09,484503.
8. Kim. Dong-Hoon (2005) ,CNC-implemented Fault Diagnosis and Web-based Remote Services, "Journal of Mechanical Science and Technology" (KSME Int. J.), Vol. 19, pp. 1095-1106.
9. Tony Boutros, Ming Liang (2007), Mechanical fault detection using fuzzy index fusion, "International Journal of Machine Tools & Manufacture" vol- 47 ,1702–1714.
10. Lautre. Nitin K. and Manna Alakesh (2006), A study on fault diagnosis and maintenance of CNC-WEDM based on binary relational analysis and expert system, "Int J AdvManufTechnol" vol-29, 490–498.
11. Huang. T. and Liao. Y. S. (2000), A wire-EDM maintenance and fault-diagnosis expert system integrated with an artificial neural network, "INT. J. PROD. RES"., VOL. 38, 1071- 1082.
12. Lanza. G, Niggeschmidt. S, Werner .P. (2009), Optimization of preventive maintenance and spare part provision for machine tools based on variable operational conditions, "CIRP Annals - Manufacturing Technology" vol-58 ,429–432.
13. Sriram Chellappan , Haghani Ali (2003), An optimization model for aircraft maintenance scheduling and re-assignment, "Enterprise Risk Management", Vol. 1,pp. 63-75.
14. VolkanovskiAndrija, Borut Mavko, Tome Bosevski, Anton Causevski, Marko Cepin (2008), Genetic algorithm optimization of the maintenance scheduling of generating units in a power system, "Reliability Engineering and System Safety" vol-93 ,757–767.
15. Abou Seraphin C., Manali Kulkarni, and Marian Stachowicz (2010), Actuated Hydraulic System Fault Detection: A Fuzzy Logic Approach, "Engineering Letters"
16. Luc Adjengue ;SoumayaYacout ; Ozlem IlkParameters (2007), Parameters Estimation for Condition Based Maintenance with Uncorrelated and Correlated Observations. "Quality Engineering", vol-19,197–206.
17. Helge Langseth , BO Henry Lindqvist, a maintenance model for components exposed to several failure mechanisms and imperfect repair. Pp 1-17.
18. W. Pujadas and F. Frank Chen (1996), reliability centered maintenance strategy for a discrete part manufacturing facility, "Computers ind.Engng", VoL 31,pp. 241-244.
19. F. FerrazJr , R.T. Coelho (2005) , Data acquisition and monitoring in machine tools with CNC of open architecture using internet. "Int J AdvManufTechnol" vol-26: 90–97.
20. Chen Zongyu , Wang L.F. , Li C.X. , Liu Y.H. (2006), The study of configuration-style CNC system based on CANBUS, "Int J AdvManufTechnol" vol- 28, 1129–1135.

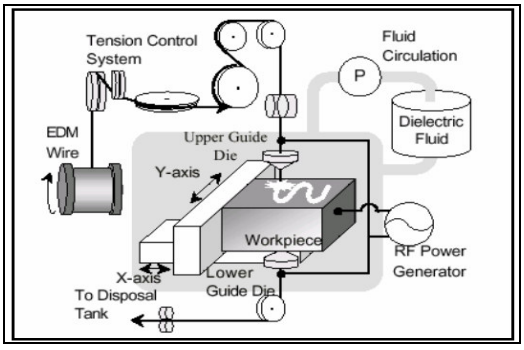

Figure 1: Wire Electrical Discharge machining system

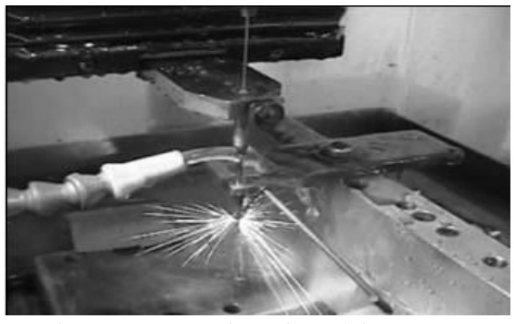

Figure 2: Generation of spark in WEDM

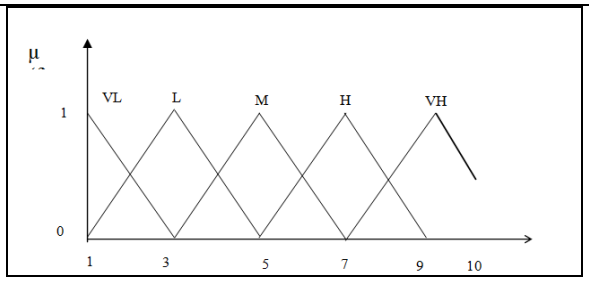

Figure 3. Triangular membership functions of input variable

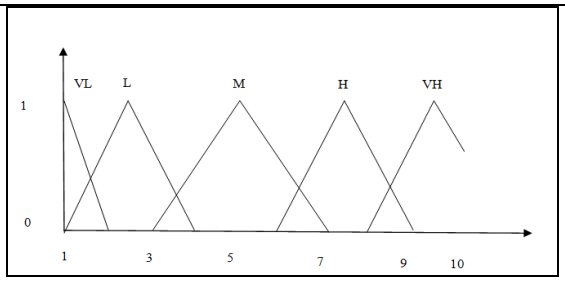

Figure 4. Triangular membership function for output variable

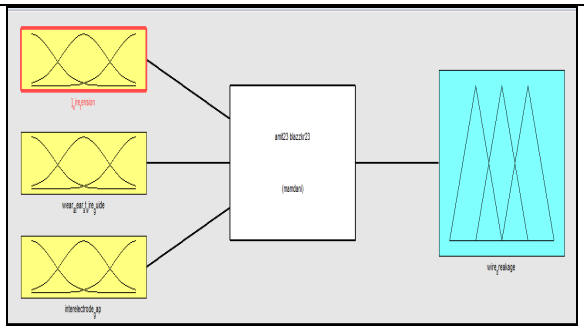

Figure 5. Fuzzy input and output

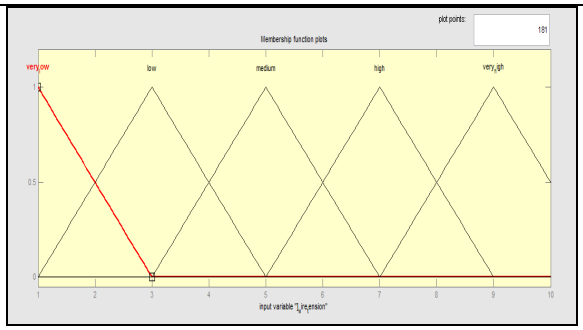

Figure 6. Input variable Membership function (wire tension)

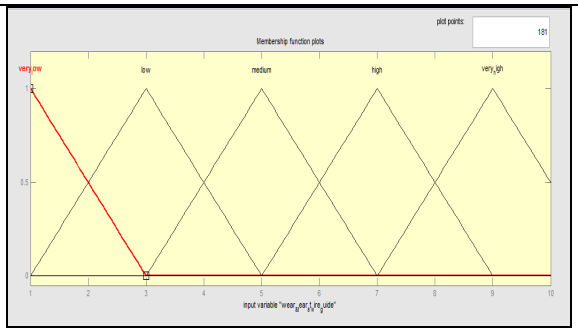

Figure 7: function for input variable (wear& tear at wire guide)

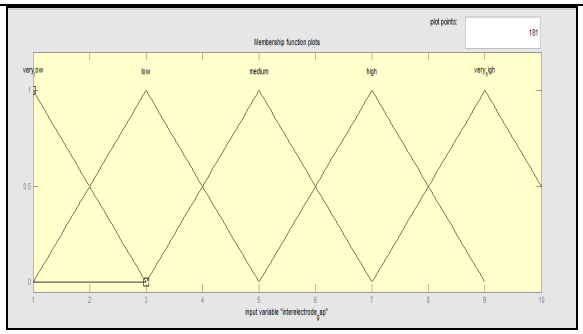

Figure 8: Membership function for input variable (inter electrode gap)

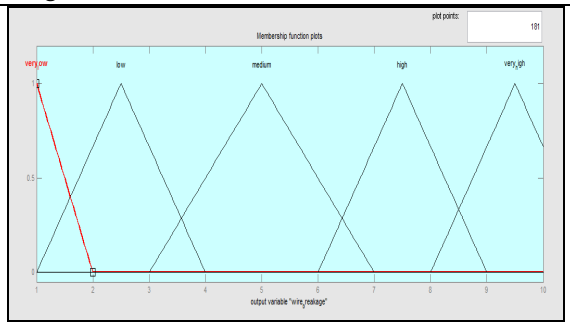

Figure 9: Output variable membership function (wire breakage)

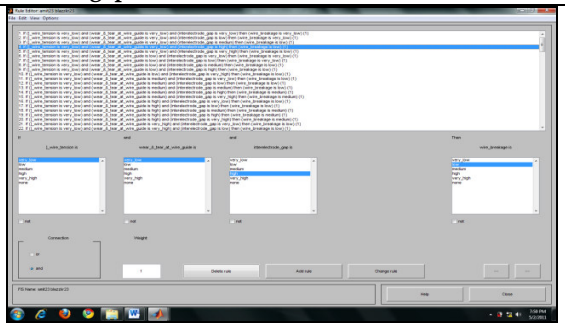

Figure 10: Fuzzy rules for wire breakage

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RESEARCH ARTICLE

Pulse Width Modulated Fuzzy Logic Controller

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ABSTRACT

This is the purpose of this paper to demonstrate that a pH neutralization process can be managed using a pulse width modulated fuzzy logic controller. pH neutralization is a process that is infamous for its extreme nonlinearity expressed in its process gaining up to 1,000 over a small area , especially as it gets close to pH 7, the set point for neutralization. Unlike the standard pulse width modulation controller that uses electronic circuits to produce the modulation of width, the pulse width modulation fuzzy logic controller has already integrated the pulse width modulation principle into its membership feature, which can then be used to regulate the mechanism of neutralization. The method of neutralization would use a basic two position pump for dosing the neutralizing agents. A strongly concentrated neutralizing agent which is 4 M HCL and NaOH is used. A comparison with two location controllers which are two stage controller, proportional controller and proportional plus derivative controller reveals that the performance of fuzzy logic controller is much higher not only in terms of the use of neutralizing agents, but also in terms of the neutralization process.

Keywords: pH control, fuzzy logic, pH neutralization, non-linear system and two position control

INTRODUCTION

Two position control or ON/OFF control play an important part in our life. Many system around us use this type of control because of its simplicity. The most common use of this type of control is in the air conditioning and refrigeration industries. There are many studies done revolving around this two position controller. An adaptive ON/ON control were used to introduce damping to the system dynamics to reduce noise, shock and vibration [1]. A predictor was also use to estimate the future system output sequences after taking accounts the whole set of future

ON-OFF input sequence over a specified number of intervals [2]. Huang [4] use a PI controller together with a pulse width modulator circuit. The latest in 1998, Choi [5] use a fuzzy logic controller to maintain the inner temperature of refrigerator inspite of environment variations.

Differ from pH control, where the set point can be in any value of pH, pH neutralization only happens when the targeted pH is pH 7 which is the neutral point. Parekh et. al (1994) says probably the pH neutralization is one of the most difficult control application. Fuzzy logic becomes very useful when the mathematical model of the process is too complex or very difficult to derive. This paper will test the fuzzy logic pulse width modulated PD controller with a high concentration of sodium hydroxide (4M) and high concentration (4M) of hydrochloric acid as a neutralizing agents. The proposed controller will only use a two position pumps which is still being widely used because of its simplicity and cheaper price. This combination of problem (high concentration and pumping limitation) makes the problem unique and very difficult case to handle.

PWM

The technique used in the proposed fuzzy logic controller is the pulse width modulation. In the normal PWM, the width of each pulse in a train is made proportional to the value of the signal at any particular point or zoning. The nth pulse can be calculated using the following equation:

$$P_{\mathrm{n}} = \int_{(n-1)\pi/N}^{n\pi N} \sin(t)dt$$

Where the width index is equal to 1. The centre of the (n)th pulse is found by:

$$C_{\mathrm{n}} = (2\mathrm{n}-1)\pi / 2\mathrm{N}$$

Where the N is the number of pulse/ half cycle.

Experiment Set-Up

Experiments are being done using a lab scale set-up. The set-up of the experiments is as in figure 1. The fuzzy logic controller main program is in the computer using BORLAND C++ language and using an interface card (PCL 818), to do the control of the system. The defuzzification technique used is based on center of gravity method. Commercially available software FULLDEK 1.1 was used to generate the fuzzy arithmetic conversion.

Design of the Fuzzy Logic Control

Fuzzy controllers have got a lot of advantages compared to the classical controllers such as the simplicity of control, low cost and the possibility to design without knowing the exact mathematical model of the process. Fuzzy logic is one of the successful applications of fuzzy set in which the variables are linguistic rather than the numeric variables. Linguistic variables, defined as variables whose values are sentences in a natural language (such as large or small), may be represented by fuzzy sets. Fuzzy set is an extension of a 'crisp' set where an element can only belong to a set (full membership) or not belong at all (no membership). Fuzzy sets allow partial membership, which means that an element may partially belong to more than one set. A fuzzy set A of a universe of discourse X is represented by a collection of ordered pairs of generic element x $\in$ X and its membership function M : X $\rightarrow$ [0 1], which associates a number A(x): X $\rightarrow$ [0 1], to each element x of X.

PWM Fuzzy Logic Controller

The PWM fuzzy logic controller being used is a rule based type controller. Membership function chosen is a triangle type and IF *x* AND *y* THEN *z* rules were used to implement this control. The antecedents to the fuzzy logic controller are error and error trend, whereas the consequences will be the act of controlling the dosing pumps of NaOH and Hcl. Membership functions for all the inputs and output parameters use for controlling the pH processes are as in fig II, III and IV.

Both of the dosing pumps will only have two position that is open and close. Although there are two pumps to be control there is only one membership function needed. This is because the positive parts of the function will be assign for NaOH pumping and the negative parts is for Hcl pumping. The controller will manipulate the duty cycle of the pumps to have an optimum effect on the process exactly like a pulse width modulator operates. This can be illustrated in figure V. Duty cycle of the pump used were 100% working, 8% working and 4% working. The duty cycle of the pumps will response accordingly to the ph values being monitored used in the decision matrix. The rules matrix used is as in TABLE 1.

RESULTS AND DISCUSSION

The result of the proposed controller is shown in FIGURE VI. This is then comparing to the other conventional Fuzzy PD controller, which is shown in FIGURE VII. The process neutralization is smooth and there is no overshoot or under shoot in FIGURE VI unlike in FIGURE VII, the neutralization process keep on overshoot and undershoot for a couple of times. The time taken by the proposed controller is also shorter.

CONCLUSION

We have presented that the proposed PWM fuzzy logic controller has been able to control the pH neutralization process very well even by using high concentration of acid and two position dosing pumps. Through the use of PWM results shown that the proposed controller is very-very much improvement from the existing fuzzy logic controller. This directly reduced the amount of neutralizing agents used and as a whole reduces the operating cost of the treatment system.

REFERENCES

1. Hung, J, Y. & Hodel, S. 1990. Adaptive control to minimize shock in ban/bang systems.
2. Golob, M., Tovornik, B. & Donlagic, D. 1992. Comparison of the self-tuning ON-OFF controller with the conventional switching controller. IEEE conference on Control applications,
3. Advantech Co., Ltd. 1993. PCL-818: High-performance DAS card with programmable gain. Ed. Ke-3 Taiwan: Advantech Co., Ltd.
4. Huang, X. & Benton, R, D. 1994. Computer based temperature controller in an energy-conservative manner.
5. Choi, B., Han, S. & Hong, S. 1998. Refrigerator temperature control using fuzzy logic and neural network.
6. D'Souza, A.F. 1988. Design of control systems. New Jersey: Prentice Hall, Inc
7. Franklin, G.F., Powell, J.D. & Workman, M. 1998. Digital Control of Dynamic Systems. 3rd Edition. California: Addison-Wesley Longman, Inc.
8. Kaufmann, A. & Gupta, M.M. 1991. Introduction to fuzzy arithmetic theory and applications. New York: Van Nostrand Reinhold.

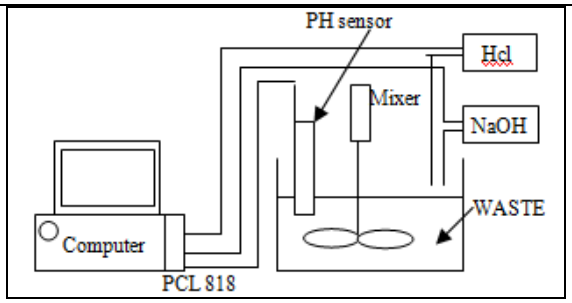

Figure 1.Experiment set-up

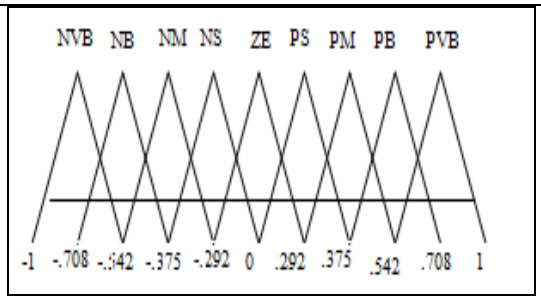

Figure 2. Membership function of error

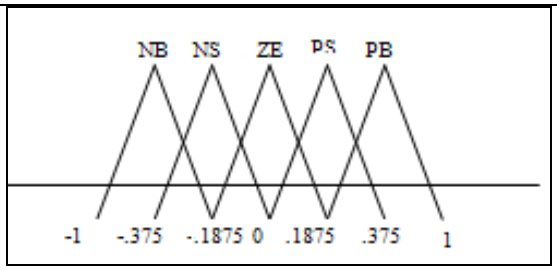

Figure 3. Membership function of trend

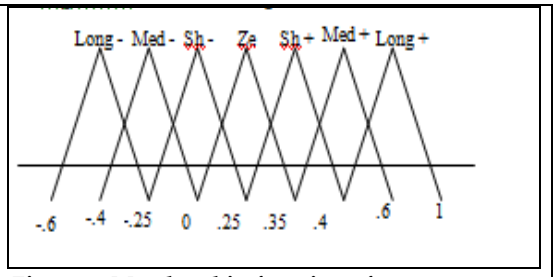

Figure 4. Membership function of pumps

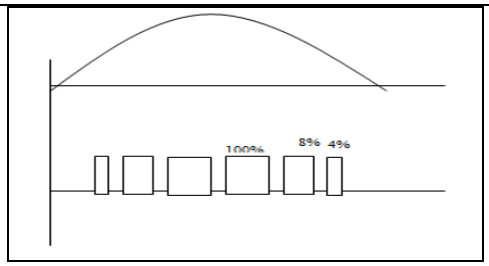

Figure5. Illustration of PWM FLC

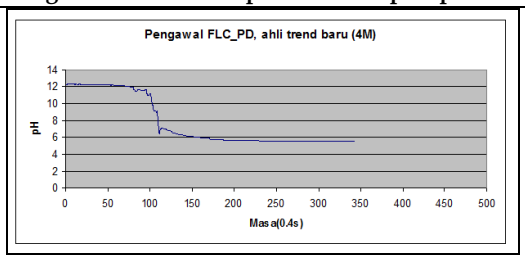

Figure 6. PWM Fuzzy logic controller

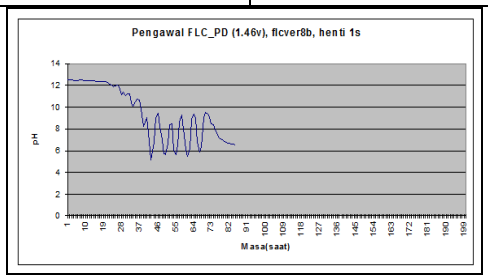

Figure 7. Fuzzy logic PD controller

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RESEARCH ARTICLE

Automatic Tool Condition Monitoring

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ABSTRACT

Tool Condition Monitoring (TCM) is a very important aspect to maintain quality of products manufactured in any machining process. This chapter presents a general overview of tool condition monitoring systems and techniques. Real-time control of the tool state is one of the most critical strategies to build in the automated cutting processes. In this method, reducing overall machining time by preventing damage in machine tools is easy. Since tool wear has a direct impact on the consistency of the machined components, online tool wear control is one of the most critical manufacturing challenges. The main aim of the work is to develop an automatic tool condition monitoring system. This system will help us to monitor the tool wear state continuously. This system will help to monitor the cutting tool in real time and, during metal cutting, it would be able to recognize most or all forms of tool anomalies. Hence it has been widely acknowledged that a better solution lies in the form automatic tool condition monitoring which could without human assistance and/or interruption recognize most or all forms of tool abnormalities during metal cutting.

Keywords: Tool condition monitoring, Tool wear

INTRODUCTION

Today, this aim has already penetrated research areas and the subject is now popularly known as automated 'Machin e State Monitoring (TCM).Manufacturing equipment has experienced major improvements in the machining industr y in the recent years. One of the most significant developments has been the trend towards cost savings through various means like reduction in staff numbers while at the same time desiring to improve product quality and reduce production time. In order to achieve the goal of automation-optimization, one of the major obstacles has been the ability to reliably detect tool wear or failure on-line. The condition of the cutting tool has to be monitored

continuously in order to replace it at appropriate time, for which some indication is required. Traditionally, tool condition monitoring has been undertaken by machine operators themselves. Based on his/her experience or using some mathematical models of the cutting process, the operator would change the tool when he/she judged it to be no longer capable of performing satisfactorily. These methods were not able to detect any sudden failure of the cutting tool or the onslaught of any failure mechanism. And these methods did not take into account the complex and diverse nature of the metal cutting operation. Thus the cutting tools were either underutilized or over utilized. To avoid this problem various types of sensory signals have been used to evaluate the condition of the cutting tool.

Tool Condition Monitoring Techniques

The need for monitoring in a metal cutting process encompasses monitoring the machine and cutting process, cutting tools and work piece to ensure optimum performance of the system. The lack of a tool condition monitoring system (TCMS) can lead to excessive power take-off, inaccurate tolerances and uneven work piece surface finish, sometimes damage to the machine tool and also injury to the operator. Research is going on for the past several years for the development of a reliable TCMS. One of the primary reasons for the lack of industrial application of TCMSs is due to the fact that these systems have been developed mainly based on mathematical models, which require huge amounts of empirical data. The nature and characteristics of the utilized sensor signals in general, tend to be stochastic and non-stationary and therefore difficult to model. It poses a practical problem, because of the complex nature of a typical metal cutting process, limiting the precision and control of the cutting process. There is a need for the TCMS to be capable of diagnosing and identifying the fault and to possibly isolate or respond with remedial action within a prescribed response time. Major work directions aimed at increasing efficiency, costeffectiveness and cost savings in big batch automated production focus on noise, tool break identification and control of wear cutting equipment.
The monitoring of tool wear and failure necessitates the development of very sensitive, accurate and reliable methods, which may be classified as being either 'direct' or 'indirect' methods. Fig. 1 shows the various methods of tool wear monitoring.

DIRECT METHODS

These methods generally involve taking measurements associated with the volumetric loss of the cutting tool material. They tend to be 'off-line' techniques, since the measurement can only be taken when the tool is out of cut. The two major disadvantages associated with offline techniques are:

- They can be very time consuming from production rate standpoint and
- The onslaught of premature cutting edge failure while tool is actually in cut cannot be detected.

Indirect methods

The shortcomings and difficulties in the implementation of direct methods have made researchers attempt to detect tool wear in-process by measuring parameters which can be closely correlated with tool wear.

Tool Wear/Failure

Failure of a cutting tool has occurred when it is no longer capable of producing parts within required specifications. Every tool, when put to use is subjected to wear after certain machining time. This is called gradual or progressive wear of the tool. During gradual wear, the tool will reach its limit of life by either flank wear or crater wear. Flank wear involves wear on the nose and the primary cutting edge with its accompanying notch. These are classified as regular wear, as they are always present in a machining operation and have 'regular' cutting time related growth characteristics. The other types of tool wear are classified as irregular tool wear phenomena and can generally be avoided by proper selection of tool material and cutting conditions. Breakage, fracture, chipping come under this category. Fracture occurs more easily in brittle tools under interrupted cutting conditions, causing not only a complete failure, but sometimes a small chipping of the cutting edge. Wear loss may be treated by replacing the instrument regularly, but cutting edge fracturing or chipping cannot be handled this way, as it typically happens as a disastrous operation. Illustration. 2 Highlights major tool wear / failure forms.

EXPERIMENTAL WORK

Abrasive wear occurs when hard inclusions of work material or escaped tool particles scratch the flank and work piece as they move across the contact area. The abrasive wear is proportional to the sliding velocity and the cutting force.

The abrasive wear can be modeled as-

$$\frac{dw}{dt} = \frac{A}{H} \propto \frac{F_f}{V.f} \propto V_s \qquad (1)$$

Where,

A= Abrasive wear constant

H= Cutting tool material hardness

F_f= Normal cutting force

V= Cutting speed

f= feed rate

V_S= Sliding velocity

Although abrasive wear mechanism is predominant in flank wear, some diffusion wear also exists. Diffusion takes place when the molecules gain sufficient energy to leave their original position. Hence activation energy too comes into the picture.

The diffusive wear rate can be modeled as-

$$\frac{dw}{dt} = B.\exp\left(-E/R.T_f\right) \qquad (2)$$

Where,

B=Diffusive wear constant

E=Activation energy

R=Universal gas constant

T_f=Temperature in the tool flank zone

The total wear rate is given by-

$$\frac{dw}{dt} = \frac{A}{H} \propto \frac{F_f}{V.f} \propto V_s + B.\exp\left(-\frac{E}{R.T_f}\right) \qquad (3)$$

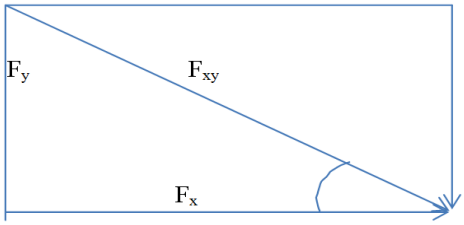
We need to calculate the values of A and B. Equation 3 is an equation with two variables. Hence we need to develop at least two equations to find the out the values of the two variables. So we need to run the experiment at least twice and get two values of wear rate. This will give us two equations which may be like-

10=2A+4B &20=5A+7B

where 10 &20 are wear values. Now we have two equations and two variables. It can be easily solved to get A & B.

Calculation of F_f(normal cutting force)

The forces in the different directions can be resolved as shown below



$$F_{xy} = \sqrt{(F_x^2) + (F_y^2)} \quad (4)$$

And, $\tan\theta = \frac{F_y}{F_x}$ (5)

And, $F_f = F_{xy} \times \cos(\gamma - \theta)$ (6)

Where, γ is the side cutting edge angle (here γ=45^0).

Calculation of sliding velocity(V_s)

$$V_s = \frac{V.\sin\phi}{\cos(\phi \quad \alpha)} \quad (7)$$

Where V= Cutting speed (m/sec)

$$V = \frac{\pi.D.N}{1000} \quad (8)$$

Where,
D = work piece diameter & N=rpm
Now as we are focusing on oblique cutting, the rake angle and the shear angle will be replaced by the effective rake angle and the effective shear angle.
Effective rake angle (α_e)-

$$\alpha_e = \tan^{-1}[\tan\alpha_s.\sin\psi + \tan\alpha_b.\cos\psi] \quad (9)$$

Where,
α_s= side rake angle
α_b= back rake angle and, ψ=chip flow angle
Calculation of chip flow angle-

$$\psi = \tan^{-1}(\tan i.\tan\alpha_n) \quad (10)$$

Where, α_n =normal rake angle
Calculation of I (angle of inclination)-

$$\tan i = \cos\gamma.\tan\alpha_s - \sin\gamma.\tan\alpha_s \quad (11)$$

Where, γ= cutting edge angle
Calculation of α_n (normal rake angle)-

$$\tan\alpha_n = \cos\gamma.\tan\alpha_s + \sin\gamma.\tan\alpha_b \quad (12)$$

Where, γ= cutting edge angle
Calculation of effective shear angle(ϕ_e)-

$$\varphi_e = \tan^{-1}\left[\frac{\left(\frac{V_c}{V}.\cos\alpha_e\right)}{1 - \left(\frac{V_c}{V}\right).\sin\alpha_e}\right] \quad (13)$$

Where,
V_c= chip velocity
v= uncut chip velocity
And α_e= effective rake angle
Now,

$$\frac{V_c}{V} = \frac{\frac{t_1}{t_c}\cos\alpha_n}{1-\frac{t_2}{t_c}\sin\alpha_n} \qquad (14)$$

Experiments

1.Cutting conditions are as follows (Fig.3)

N= 250 rpm
Depth of cut= 0.5 mm
Feed= 0.04mm/rev.
Time= 2 min.
Work piece diameter= 23.30 mm
Chip thickness, t_c=0.21 mm
The forces measured by the dynamometer are as follows
F_X= 5N
F_Y= 26.123 N

2.Cutting conditions are as follows (Fig.4)

N= 250 rpm, Depth of cut= 0.5 mm, Feed= 0.04mm/rev. and Time= 1.5 min.
Work piece diameter= 23.30 mm
Chip thickness, t_c=0.21 mm
The forces measured by the dynamometer are as follows
F_X= 6 and F_Y= 19.043 N
The values of the abrasive wear constant A and diffusive wear constant B is calculated and is obtained as follows-
A= -4.92×10^{-9}
B= 14.93

3.Cutting conditions are as follows (Fig.5)

N= 840 rpm, Depth of cut= 1 mm, Feed= 0.04mm/rev. and Time= 2 min.
Work piece diameter= 27.30 mm
Chip thickness, t_c=0.21 mm
The forces measured by the dynamometer are as follows
F_X= 6N and F_Y= 136.719 N
The average flank wear measured by the microscope is 0.207 mm.

4. Cutting conditions are as follows (Fig.6)

N= 840 rpm, Depth of cut= 1 mm, Feed= 0.04mm/rev. and Time= 1.5 min.
Work piece diameter= 25.30 mm, Chip thickness, t_c=0.21 mm
The forces measured by the dynamometer are as follows
F_X= 7N and F_Y= 129.883 N
The average flank wear measured by the microscope is 0.197 mm

CONCLUSIONS

In this report, a method for cutting-tool condition monitoring on lathe machine is define, the method being focused on measuring the axial force. From the edge test, one may draw the following conclusions.

- The axial stress, measured at a set pressing distance, and the cutting tool's flank wear are closely related.
- Instead of measuring the real flank wear the force criterion may be used to determine the cutting-tool situation.
- Much work needs to be undertaken to successfully incorporate automatic device failure sensing in scalable manufacturing and better understand the interactions between these factors and the failure of the devices. F_x and F_Y has been found to be the best feature correlated with flank wear.

REFERENCES

1. Chaari, R.; Abdennadher, M.; Louati, J.; Haddar, M. Modelling of the 3D Machining Geometric Defects Accounting for Workpiece Vibratory Behaviour. International Journal of Simulation Modelling, 10, 2(2011), pp. 66-77.
2. Barkallah, M.; Louati, J.; Haddar, M. Evaluation of Manufacturing Tolerance Using a Statistical Method and Experimentation. International Journal of Simulation Modelling, 11, 1(2012), pp. 5-16.
3. Sadílek, M.; Čep, R.; Budak, I.; Soković, M. Aspects of using tool axis inclination angle. Strojniski vestnik – Journal of Mechanical Engineering. 57, 9(2011), pp. 681- 688.
4. Salgado, D. R.; Alonso, F. J. Tool wear detection in turning operations using singular spectrum analysis. Journal of Materials Processing Technology. 171, 1(2006), pp. 451- 458.
5. G. Wang, Y. Yang and Z. Li, "Force sensor based tool condition monitoring using a heterogeneous ensemble learning model", Sensors, vol. 14, no. 11, pp. 21588-21602, 2014.
6. C. H. Lauro, L. Brandão, D. Baldo, R. A. Reis and J. P. Davim, "Monitoring and processing signal applied in machining processes—A review", Measurement, vol. 58, pp. 73-86, Dec. 2014.
7. M. Malekian, S. S. Park and M. B. G. Jun, "Tool wear monitoring of micro-milling operations", J. Mater. Process. Technol., vol. 209, no. 10, pp. 4903-4914, 2009.
8. E. Jantunen, "A summary of methods applied to tool condition monitoring in drilling", Int. J. Mach. Tools Manuf., vol. 42, no. 9, pp. 997-1010, 2002.
9. B. Sick, "On-line and indirect tool wear monitoring in turning with artificial neural networks: A review of more than a decade of research", Mech. Syst. Signal Process., vol. 16, no. 4, pp. 487-546, 2002.

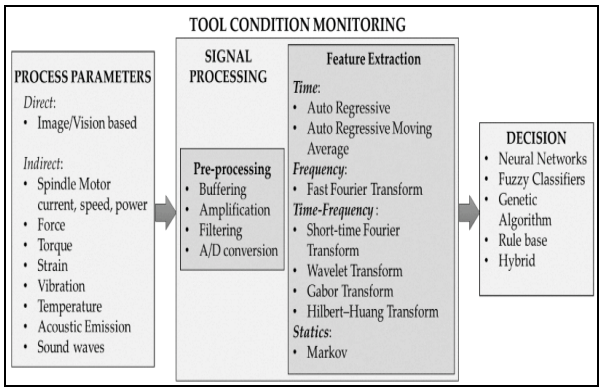


Figure. 1 Various Methods of Tool Wear Monitoring

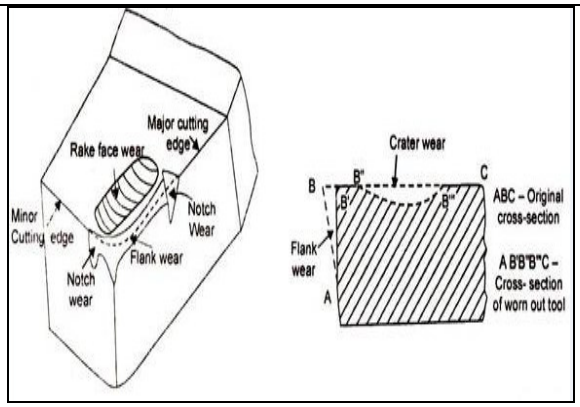


Figure 2 Tool wear phenomenon and Crater wear

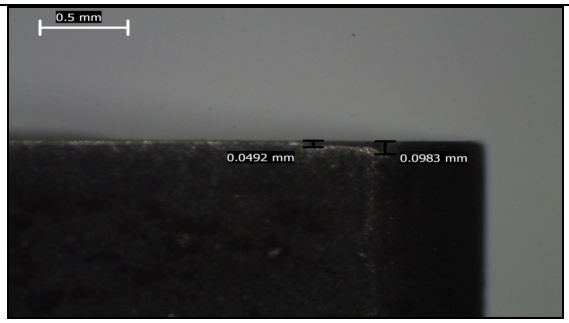


Figure 3. The average flank wear measured by the microscope is 0.0492 mm.

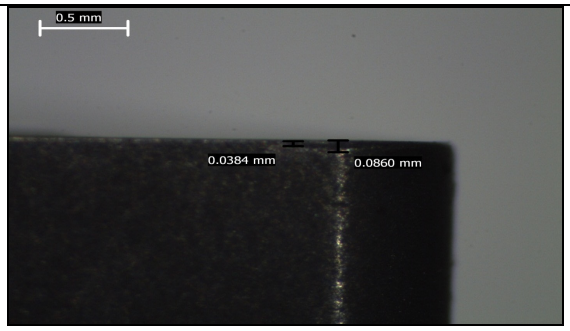


Figure 4 The average flank wear measured by the microscope is 0.0384mm

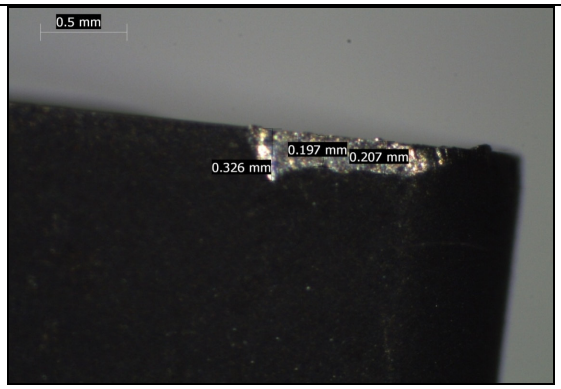


Figure 5 Flank wear measured by the microscope

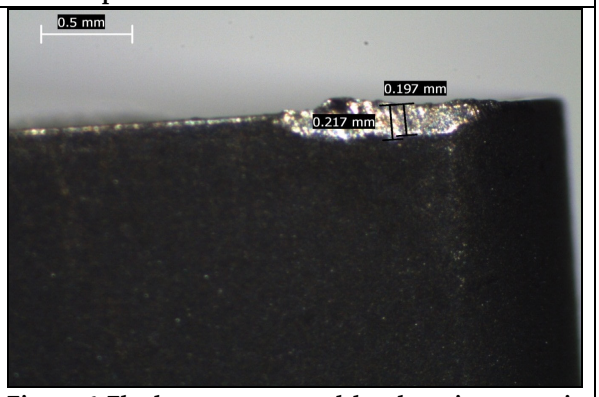


Figure 6 Flank wear measured by the microscope is 0.197 mm

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RESEARCH ARTICLE

Back Engineering and Rapid Prototyping in Casting Process

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ABSTRACT

Back or Reverse engineering is the practice in which a product design can be analyzed or re-created by means of a physical part or mock up. In the automotive industry, reverse engineering of spare parts is evident. Parts that are dropped or quite challenging to obtain may be recreated in a limited time, guaranteeing consumer service. Again Rapid prototyping (RP) has a significant influence on the worldwide manufacturing sector. The combination of reverse engineering and rapid prototyping is used to rapidly bring the product into the market by overcoming a persistent gap between concept and manufacturing. The paper examines possible uses for metal casting, as well as an effort to test the technology's limits.

Keywords: CAD, Rapid Prototyping, Metal Casting, FDM, Reverse or Back Engineering

INTRODUCTION

The goal reverse engineering to quickly and successfully sustain and/or improve the production skills of today using the equipment of yesterday, before tomorrow arrives. Reverse engineering is the equivalent to forward technologies. To modify or reproduce the design aspect of the product. It can also be defined as the process of duplicating an individual component by collecting the physical measurements of the components. Reverse engineering is typically undertaken to modify the system for improved maintenance or to make a replica of a system without reference to the original version. The development of their CAD models is required to facilitate the operations of these physical models in computer-aided manufacturing (CAM). RE is the easiest way to transfer the data through any operating device. The aim of reverse engineering an object is to effectively create an object's 3D CAD model which can be used

to possibly model parts where there is no CAD model. To create clean, smooth 3D models which are noiseless and holes-free. It requires a solid, reliable image acquisition device that can acquire data in a reasonable time frame with a high degree of accuracy. The output is converted data, represented as 3D reconstructions.

Reverse Engineering Process

In general terms, reverse engineering is a series of four different stages preceded by a pre-screening process, each stage building on previous stage performance. In general, engineers and researchers follow the following four-stage process in order to reverse engineer a product or component of a system:

Stage 1: Assessment & Verification
Stage 2: Evaluation and Verification
Stage 3: Design Verification
Stage 4: Implementation of project

Application of Manufacturing Process through Rapid Prototyping

Reverse engineering is a method used where an current part needs to be replicated and prototypes are unavailable. To receive new data, the part must be weighed and redrawn, as well as to allow the item to be re-manufactured. This can be achieved in many ways, from actually calculating the measurements with calipers to capturing the data to be redrawn, to the advanced methods of converting x-ray imaging or 3D LASER scanning images into CAD data files today. The entire RP method creates structures by creating very thin cross-sections of the part before the solid physical component is executed. By this process of three-dimensional construction to forming and piling together, basically two-dimensional slices.

Fundamentals of RP System

There are a few common features to all prototypes developed using current and evolving RP processes. While at present they are more than 20 vendors for RP systems, the method used by each vendor can generally be classified into the following categories: photo-curing, cutting and gluing / joining, melting and solidifying / fusing and joining / binding. Photo-curing can be further divided into single laser beam, double laser beam and masked lamp categories.

Experimental Procedure

By connecting Solid Works to a 3D Digitizer or Coordinate Measuring System (CMM), Rev Works opens the door to dramatically improved flexibility that allows the design purpose of the pieces to be captured quicker. Equipped with Catalyst tools, the computer system converts / slices the 3D CAD model into STL (Stereo lithography) format as well as provides support to the framework for new components.

Sand Casting and FFDM Process

The method of casting sand is fairly easy, and the sand is created molds and parts made of cast metal are fairly easy. However, it can be time consuming to manufacture the patterns for making the sand molds. Applying FDM to the sand casting process decreases design creation time to speed the receipt of sample or sand cast pieces from manufacturing.

Process Overview

In the casting of sand the tool has two parts. The cope is the tool's top-side. Depending on the form of metal being poured, it can include sprue, lock, vent, risers, and filters. Depending on the form of metal being poured, it can include sprue, lock, vents, risers, and filters. The drag usually features runners, gates, and wells. The loose cores, often made of clay, are placed in the cope and dragged where undercuts are present, or where there are hollow areas in the cast component. The process begins with the design of the cast part and the delivery of metal routes within the container. The compacted sand is bound together by binders that are uses in clay (green sand), or chemical agents (dry sand).Molten metal is shed through the sprue onto the container. It flows into the part cavity via the runners

and gates. When the metal cools and shrinks, the metal also fills the riser, which serves as a tank that helps to feed the component cavity. The metal is then allowed to cool and solidify, and the pieces of the sand are torn apart.

CONCLUSION

For centuries casting of sand has been used with no alteration to the simple method. It is concluded that developing a larger scale market tools produced using layer manufacturing techniques requires two things: technical developments, especially in terms of precision, surface finishing and durability; and increased awareness of manufacturing volume economies and the importance of tools within that economic frame work. Rapid prototyping (RP) will influence the design process and this article illustrates the whole manufacturing process for the product. The speed and versatility of RP technologies reduced the average time needed to complete the drug.

REFERENCES

1. Ingle, K. A., "Reverse Engineering". McGraw-Hill Book Company, Inc., New York, 1994. pp. 7-23.
2. Rafiq Noorani, "Rapid Prototyping: Principles and Applications," John Wiley & Sons,Inc.
3. Kenneth G. Cooper, "Rapid Prototyping Technology," Marcel Dekker, Inc.
4. Ali Kamrani and Emad Abouel Nasr, "Rapid Prototyping : Theory and Practice," Springer
5. Patri K. Venuvinod and Weiyin Ma, "Rapid Prototyping – laser Based and Other Technologies," Kluwer Academic Publishers
6. Rapid System Prototyping, 1999. IEEE International Workshop, Jul 1999, Clearwater, FL, USA
7. The Authority on Emerging Technologies for Design Solutions [online]. Available:http://www.elecdesign.com/Articles/Index.cfm?AD=1&Article ID=11966 ,Jan 2006
8. William B. Thompson, Jonathan C. Owen, and H. James de St. Germain Technical report on "Feature-Based Reverse Engineering of Mechanical Parts", University of Utah Technical Report UUCS-95-010 (revised), November 6, 1995
9. Varady T.; Martin R.R.; Cox J., "Reverse engineering of geometric models--an introduction," Computer-Aided Design, Volume 29, Number 4, April 1997 , pp. 255-268(14); Publisher: Elsevier
10. New Product Development Consulting Services, http://www.npd-solutions.com
11. An article from the URL: http://www.chillingeffects.org
12. Bradley C.," The application of reverse engineering in rapid product development". Sensor Review Volume: 18, Issue: 2, 1998. pp. 115-120.
13. Usher M. John, Roy Utpal and Parsaei, H. R.,"Integrated Product and Process Development". John Wiley & Sons, Inc., New York, 1998. pp. 151-183.

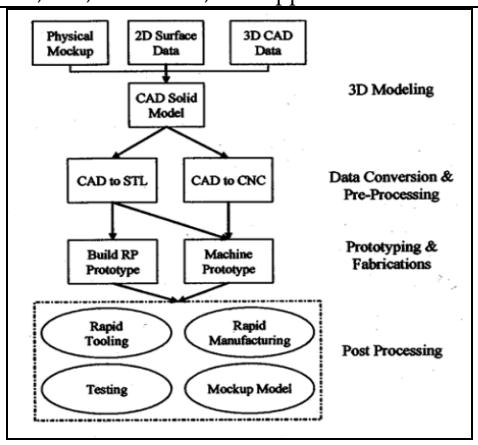

Figure 1 Generic Rapid Prototyping Process

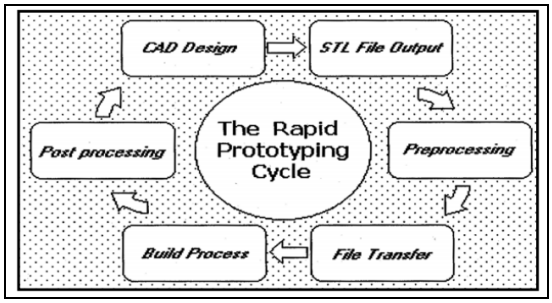

Figure 2 Function of Reverse Prototype Tool

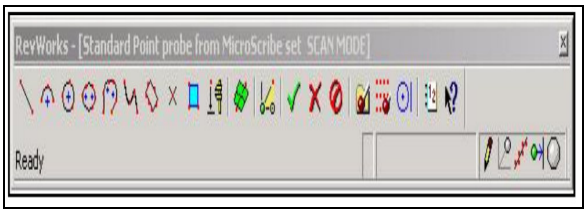

Figure 3 RevWorks Toolbar

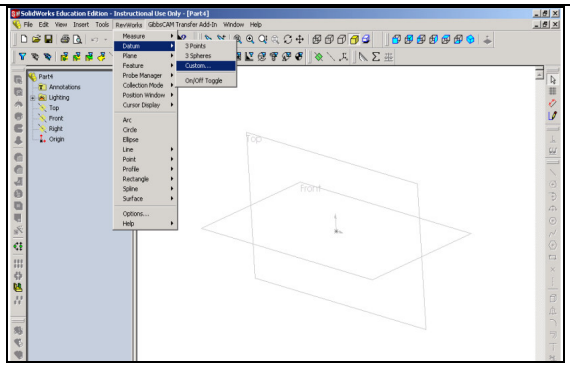

Figure 4 Data Selection from Solidworks Menu Function

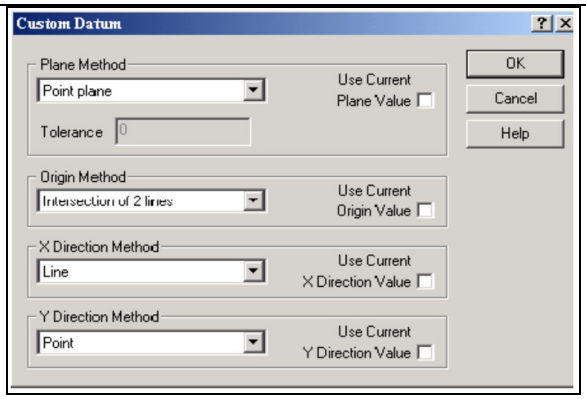

Figure 5 Menu for Datum Selection

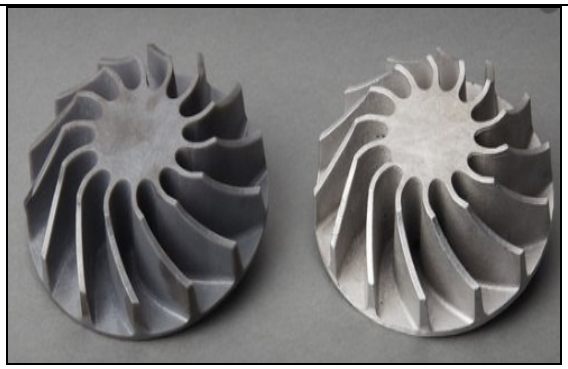

Figure 6 Comparison of Casting and ABS pattern

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RESEARCH ARTICLE

An Efficient Trajectory Planning Approach for a 6-DOF Kawasaki RS06L Manipulator using a Hybrid Cuckoo-Bat Algorithm

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ABSTRACT

This paper proposed a new hybrid cuckoo-bat algorithm which offers better solution for the optimal trajectory planning problem of robot manipulator. A Kawasaki RS06L robot manipulator with 6R configuration has been considered for illustration of the entire trajectory planning task. The 4x4 DH forward transformation matrix of the considered 6R manipulator has been calculated. The end-effector target point in terms of position and orientation coordinates is defined with definite robot workspace (specified joint limits). An error function which is a combination of both error in position and error in orientation coordinates is defined as total objective function for the optimization assignment. In order to accomplish an optimal trajectory, best cost of the error objective fitness function, algorithm convergence speed, the variation of joint angles, and the error in positions are chosen as performance parameters. The objective function has been executed using bat algorithm (BA), cuckoo-search algorithm (CS), firefly algorithm (FA), artificial bee colony (ABC) algorithm, particle swarm optimization algorithm (PSO), teaching–learning-based optimization algorithm (TLBO) and the proposed hybrid cuckoo-bat algorithm (HCB). The intermediated coordinates of locus has been found out using forward kinematics equation. The accomplished optimal trajectory results for the defined task using the new HCB algorithm have been depicted in graphical form. The effectiveness of the proposed HCB is validated by carrying out a comparative review of the acquired HCB algorithm trajectory results with that of other considered existing algorithms. The significance and the rank of the algorithms have been computed by conducting Friedman test for the mean solutions of error in positions and orientation. The comparative study of the implemented algorithms confirms that HCB executes superior than the other algorithms with less computational effort in same boundary conditions.

Keywords: Trajectory planning, optimization, heuristic optimization methods, hybrid cuckoo-bat algorithm (HCB), graphical simulation, motion analysis

INTRODUCTION

Robots are greatly being engaged for various applications in so many fields due to its flexibility, repeatability, preciseness and accuracy of performing the assigned task. The application area mostly includes the industrial robot manipulator operations such as assembly, machining, spray painting, machine loading/ unloading, welding, material handling, etc. The motive of the industries and the engineers are to carry out the process of automation effectively and accurately in less manufacturing cycle time. So the automation process needed to be optimized in terms total time i.e. manufacturing lead time (MLT) and optimal motion control. The smoothness and accuracy assigned trajectory to perform the whole operation affects the final end product precise and accuracy. So, in the context of trajectory planning and robot motion planning the execution time must be minimized in order to increase total productivity. So as to acquire smooth and accurate manipulation of the considered manipulators for the intended task, its joints parameters or variables are also must be optimized. In real time environment robot motion and trajectory planning are performed in Cartesian-space, whereas the control is performed in joint-space. Therefore, the trajectory planning problem which involves the inverse kinematics (IK) solution of robot manipulators must be optimized. And, the nature of effecting in multiple solutions while solving IK problem makes the mathematical computation more complex and difficult. The current generation researchers mostly implement the metaheuristic techniques and algorithms for faster execution of trajectory planning problem as compared to the conventional algebraic and geometric approaches. The metaheuristics methods are also providing better optimal solution to the concerned problem. In order to find solution to trajectory planning and IK problem, so many researchers have worked upon the application of soft computing methods for various defined operations. In the following section some of earlier conducted research works were explained.

Problem Definition and Objective Function

The prime objective of the trajectory planning problem is to generate an optimal trajectory (i.e. optimum trajectory length/ best cost, optimal joint angle and joint angle variation, minimum error in positions). For illustration purpose, a manipulator as shown in Figure 3 has been chosen so as to move to a specific desired target. The robot kinematic model of the chosen Kawasaki RS06L robot has been presented in the Figure 1. The specification of the Kawasaki RS06L robot model has been given in Table 1. The schematic link diagram with coordinate frame of the Kawasaki RS06L manipulator has been presented in Figure 2. The DH kinematic parameters extracted from the Figure 2 are tabulated in Table 2.

Proposed Hybrid Cuckoo-Bat Algorithm (HCB)

This section of the paper presents a brief description of the new proposed hybrid algorithm for the optimal trajectory planning problem of a Kawasaki manipulator. In order to acquire optimal solutions for the desired task, the concept of CS and BA has been merged to custom the hybrid algorithm. The optimization process do considers two objectives function i.e. one for the error in position and the other being the error for orientation. And hence, the total fitness function is the combination of both i.e. error in position (equation-18) and error in orientation (equation-19) and it is defined as by equation (21),

$$f = w_1 * f_1 + w_2 * f_2 \quad (1)$$

where, w_1 and w_2 are weighing factor. In this case equal weightage has been assigned to both position and orientation so as to obtained optimal solution for the end-effector trajectory accurately. Hence, $w_1 = 0.5$ and $w_2 = 0.5$.

The entire process of optimization of the trajectory planning problem using the developed hybrid algorithm has been presented in the Figure 5. The optimization planning begins with the inputs of kinematic parameters, the workspace and the desired target point. The feasibility of the position and orientation has been verified for the defined joint variables limits. The forward kinematics equations along with a combined objective function for position and

orientation coordinates are defined. Then the initialization of optimization algorithms is done with a random population and a set of optimization parameters such as pulse frequency, pulse rate loudness, etc. then the concept of CS algorithm has been implemented to find a local optimal solutions. Firstly, a random cuckoo i.e. set of position and orientation coordinates are chosen for evaluation of objective fitness value. And then, another cuckoo i.e. set of coordinates are picked followed by its fitness evaluation. The lower value fitness among two calculated fitness is forwarded to the next step which is termed as current best. The worst finesses among them are eliminated. The best local optimal solution viz. the current best of the CS algorithm is given as input to the bat algorithm (BA) for global optimization. In BA, new solutions are generated by updating the velocity, pulse emission rate and loudness of the local solutions obtained from CS algorithm. The new solution is checked for its efficacy in reference to the previous solution and accordingly the best are accepted to calculate the position orientation, objective fitness using forward kinematics. The best bats i.e. the optimal trajectory solutions in the terms of various performance parameters are stored in the system. The entire process is repeated until the previously defined maximum iteration is reached. The considered algorithms have been run for 500 iterations with the same population size. The values of tuning parameters used in different algorithms are given in Table 3. The algorithm tuning parameters are denoted as given below,

β = Levy flight factor for CS,
p_a = probability factor (Discover rate of ailing eggs),
γ = Light Absorption Coefficient, β_0 = Attraction Coefficient Base Value,
α = Mutation Coefficient, α-damp = Mutation Coefficient Damping Ratio,
δ = Uniform Mutation Range, w = Inertia weight,
α-damp = Inertia Weight Damping Ratio, C1 = Personal Learning Coefficient,
C2 = Global Learning Coefficient.

In ABC, the number onlooker bees are equal to number of employed bees and acceleration coefficient is 1. In BA frequency ranges from 0 to 2. The considered algorithms are run for 10 independent runs and the best results are picked.

RESULTS

Results Obtained with Hybrid Cuckoo-Bat Algorithm (HCB)

The convergence of HCB algorithms at different runs has been presented in Figure 6, where, R's represent the runs of algorithm execution. As it can be observed that at R24 run, the algorithm is resulting in best solution of the fitness value. Figure 7 depicts the best cost plot of the proposed HCB algorithm. The variations of joint angle θ_1, θ_2 and θ_3 have been shown in Figure 8. Similarly, the variations of joint angle θ_4, θ_5 and θ_6 have been shown in Figure 9. The position and orientation errors in different directions obtained from HCB method are presented in Figure 8 and Figure 9 respectively.

The error in position in X-direction presented in Figure 19 indicates that the error in HCB is least showing that the best solution accuracy as compared to other methods. Here, FA, TLBO and PSO are providing good results whereas CS, BA and ABC perform the worst. The error plot as shown in Figure 20 shows that the error in Y-direction obtained with HCB is least while CS, BA, FA, ABC and PSO are resulting in inaccurate results. The result of HCB is as good as of the TLBO. Figure 21 reveals that the error in position for Z-direction for HCB, BA, ABC and TLBO are lesser as compared to other. Similarly, the error in orientation value in X-direction for all algorithms has been presented in Figure 22. It indicates that HCB, ABC and BA are yielding optimum and accurate solution relative to other methods. Here, CS, FA and TLBO are worst performer.

The trajectory solution results of mean error in positions and orientations for the defined objective functions of 10 runs have been taken to check the statistical significance of all techniques. In order to verify the effectiveness of the HCB method, the comparative student's t-test of results of two groups/methods at once has been conducted using Friedman ANOVA test [36]. Sometimes, for more than two groups results the t-test leads to improper results at constant confidence interval, $\alpha = 0.05$ and the results comes as at this significance level, the populations are different. The Friedman test works on the concept of accepting/rejecting a predefined null hypothesis and check whether the input parameters are significant or not.

The Friedman ANOVA test is performed in OriginPro 2016 software and the output results in terms of p-value at significance level, $\alpha = 0.05$ has been presented in Table 3. It can be observed from the results of Table 3 that the p-value of HCB-TLBO and CS_TLBO are 0.52709 and 1 respectively. This confirms that the solutions of HCB and TLBO are not significantly different. The p-value 1 indicates that the results of CS and TLBO are same. Similarly, the p-value of CS-HCB, CS-FA, HCB-FA, ABC-PSO, PSO-FA combinations shows that there is no statistical difference in their solutions. It is concluded from the overall p-value of algorithms solutions in the Table 3 that BA, FA, ABC, and PSO are producing results having more statistical difference relative to CS, HCB and TLBO.

Furthermore, the CS, HCB and TLBO techniques have provided better results relative to other methods. There is very small difference in algorithms tendency in finding the worst and mean solutions. Therefore, in order to quantify the algorithms performance, Friedman rank test [36] has been conducted for all algorithms at a time in OriginPro environment. The Friedman rank test result of mean error fitness value for the implemented algorithms has been shown in Table 4. The rank test confirms that HCB is ranked 1 followed by TLBO and CS in the 2nd and 3rd rank respectively. BA and ABC are ranked in the last in this test. It can also be seen that the difference in the Friedman rank of HCB, TLBO and CS is minimal i.e. 19, 23 and 24 respectively. The Friedman rank of PSO, ABC and BA are 52, 60 and 62 respectively which are much lower in rank than the proposed HCB algorithm with Friedman rank 19. Similarly, the mean rank of HCB is 1.9 which is much higher than PSO, ABC and BA having mean rank of 5.2, 6.0 and 6.2 respectively. The mean rank of TLBO and CS are 2.3 and 2.4 respectively which have minimal difference with that of HCB. From the above test it can be concluded that HCB is performing best and BA is offering worst solutions. The familiar algorithms like TLBO and PSO are the next best methods after HCB.

CONCLUSION

This paper proposes a hybrid cuckoo bat algorithm (HCB) for the trajectory optimization problem for a simple 6R Kawasaki RS06L robot manipulator. The existing algorithms such as CS, BA, FA, ABC, PSO and TLBO algorithms are also used to solve the trajectory optimization problem for the same manipulator with same set of constraints. The optimized trajectory results obtained from HCB in terms of performance parameters such as best cost, joint angle variations, error in positions and orientations has been presented. The results of HCB were compared with that of the CS, BA, FA, ABC, PSO and TLBO. The results of simulation verify that HCB is producing optimal trajectory with minimum error in positions and orientations. The variations in joint angles obtained through HCB are least as compared to other algorithms. On the other hand, CS and TLBO are performing well for some cases whereas the new hybrid algorithm performs consistently better in all cases of evaluation of optimal performance parameters. The Friedman ANOVA test confirms that the results obtained for mean solution of the error fitness function are not significantly different. The other two are CS and TLBO where the results produced are of not much statistical difference. In order to verify the effectiveness of all algorithms the Friedman rank test results is also conducted which reveals that the HCB is ranked 1st among the other chosen existing algorithms. The execution/computational time is also less for HCB as compared to other algorithms (except CS) as they converge for the optimum solutions. In the overall review of algorithms HCB is performing better and BA being the worst one. Therefore, the aforementioned evaluation recommends that a better, optimal, precise and accurate trajectory planning can be performed with HCB in lesser time.

REFERENCES

1. Ayyıldız, M. and Çetinkaya, K.: Comparison of four different heuristic optimization algorithms for the inverse kinematics solution of a real 4-DOF serial robot manipulator. Neural Computing and Applications. 27(4), 825-836 (2016)
2. Gigras, Y., Jora, N. and Dhull, A.: Comparison between Different Meta-Heuristic Algorithms for Path Planning in Robotics. International Journal of Computer Applications. 142(3) (2016)
3. Kazem, B.I., Mahdi, A.I. and Oudah, A.T.: Motion planning for a robot arm by using genetic algorithm. JJMIE. 2(3) (2008)
4. Savsani, P., Jhala, R.L. and Savsani, V.J.: Optimized trajectory planning of a robotic arm using teaching learning based optimization (TLBO) and artificial bee colony (ABC) optimization techniques. In Systems Conference (SysCon), 2013 IEEE International. 381-386 (2013)
5. Savsani, P., Jhala, R.L. and Savsani, V.J.: Comparative study of different metaheuristics for the trajectory planning of a robotic arm. IEEE Systems Journal. 10(2), 697-708 (2016)
6. Rokbani, N., Casals, A. and Alimi, A.M.: IK-FA, a new heuristic inverse kinematics solver using firefly algorithm. In Computational Intelligence Applications in Modeling and Control, Springer. 369-395 (2015)
7. Cham. Aghajarian, M. and Kiani, K., 2011, November. Inverse kinematics solution of PUMA 560 robot arm using ANFIS. International Conference on Ubiquitous Robots and Ambient Intelligence (URAI), IEEE. 574-578 (2011)
8. Masajedi, P., Shirazi, K.H. and Ghanbarzadeh, A.: 3D Trajectory Planning for a 6R Manipulator Robot Using BA and ADAMS. In Information Technology Convergence Springer, Dordrecht. 807-816 (2013)
9. Hossain, M.A. and Ferdous, I.: Autonomous robot path planning in dynamic environment using a new optimization technique inspired by bacterial foraging technique. Robotics and Autonomous Systems. 64,137-141 (2015)
10. Mohanty, P.K. and Parhi, D.R.: Optimal path planning for a mobile robot using cuckoo search algorithm. Journal of Experimental & Theoretical Artificial Intelligence. 28(1-2), 35-52 (2016)
11. Klempka, R. and Filipowicz, B.:Comparison of using the genetic algorithm and cuckoo search for multicriteria optimisation with limitation. Turkish Journal of Electrical Engineering & Computer Sciences. 25(2), 1300-1310 (2017)
12. Huang, H.C., Chen, C.P. and Wang, P.R.: Particle swarm optimization for solving the inverse kinematics of 7-DOF robotic manipulators. In Systems, Man, and Cybernetics (SMC), 2012 IEEE International Conference on IEEE. 3105-3110 (2012)
13. Amouri, A., Mahfoudi, C., Zaatri, A., Lakhal, O. and Merzouki, R.: A metaheuristic approach to solve inverse kinematics of continuum manipulators. Proceedings of the Institution of Mechanical Engineers, Part I: Journal of Systems and Control Engineering. 231(5), 380-394 (2017)
14. Bayati, M.: Using cuckoo optimization algorithm and imperialist competitive algorithm to solve inverse kinematics problem for numerical control of robotic manipulators. Proceedings of the Institution of Mechanical Engineers, Part I: Journal of Systems and Control Engineering. 229(5), 375-387 (2015)
15. Reynolds, A.M. and Rhodes, C.J.: The Lévy flight paradigm: random search patterns and mechanisms. Ecology. 90(4), 877-887 (2009)
16. Yang, X.S. and Deb, S.: December. Cuckoo search via Lévy flights. In Nature & Biologically Inspired Computing, 2009. NaBIC 2009. World Congress on IEEE. 210-214 (2009)
17. Yang, X.S.: A new metaheuristic bat-inspired algorithm. In Nature inspired cooperative strategies for optimization (NICSO 2010) Springer, Berlin, Heidelberg. 65-74 (2010)
18. Yang, X.S.: Nature-inspired metaheuristic algorithms. Luniver press. (2010)
19. Yang, X.S.: Firefly algorithms for multimodal optimization. In International symposium on stochastic algorithms, Springer, Berlin, Heidelberg 169-178 (2009)
20. Yang, X.S.: Firefly algorithm, Levy flights and global optimization. In Research and development in intelligent systems XXVI, Springer, London. 209-218 (2010)

21. Aderhold, A., Diwold, K., Scheidler, A. and Middendorf, M., 2010. Artificial bee colony optimization: a new selection scheme and its performance. In Nature Inspired Cooperative Strategies for Optimization (NICSO 2010), Springer, Berlin, Heidelberg 283-294 (2010)
22. Karaboga, D.: An idea based on honey bee swarm for numerical optimization Technical report-tr06, Erciyes university, engineering faculty, computer engineering department. 200 (2005)
23. Akay, B. and Karaboga, D.: Parameter tuning for the artificial bee colony algorithm. In International Conference on Computational Collective Intelligence, Springer, Berlin, Heidelberg. 608-619 (2009)
24. Karaboga, D. and Akay, B.: A comparative study of artificial bee colony algorithm. Applied mathematics and computation. 214(1), 108-132 (2009)
25. Karaboga, D. and Basturk, B.: A powerful and efficient algorithm for numerical function optimization: artificial bee colony (ABC) algorithm. Journal of global optimization. 39(3), 459-471 (2007)
26. Engelbrecht, A.P.: Fundamentals of computational swarm intelligence. John Wiley & Sons (2006)
27. Rini, D.P., Shamsuddin, S.M. and Yuhaniz, S.S.: Particle swarm optimization: technique, system and challenges. International journal of computer applications. 14(1), 19-26 (2011)
28. Kim, J.J. and Lee, J.J.: Trajectory optimization with particle swarm optimization for manipulator motion planning. IEEE Transactions on Industrial Informatics. 11(3), 620-631 (2015)
29. Kwak, D.J., Choi, B. and Kim, H.J.: Trajectory optimization using virtual motion camouflage and particle swarm optimization. In International Conference on Intelligent Robotics and Applications, Springer, Berlin, Heidelberg. 594-604 (2013)
30. Ghalia, M.B.: Particle swarm optimization with an improved exploration-exploitation balance. In Circuits and Systems, 2008. MWSCAS 2008. 51st Midwest Symposium on IEEE. 759-762 (2008)
31. Rao, R.V. and Patel, V.: An improved teaching-learning-based optimization algorithm for solving unconstrained optimization problems. Scientia Iranica. 20(3), 710-720 (2013)
32. Rao, R.V., Savsani, V.J. and Balic, J.: Teaching–learning-based optimization algorithm for unconstrained and constrained real-parameter optimization problems. Engineering Optimization. 44(12), 1447-1462 (2012)
33. Rao, R.V., Savsani, V.J. and Vakharia, D.P.: Teaching–learning-based optimization: an optimization method for continuous non-linear large scale problems. Information Sciences. 183(1), 1-15 (2012)
34. Rao, R.V. and Savsani, V.J.: Mechanical design optimization using advanced optimization techniques. Springer Science & Business Media (2012)
35. Groover, M.P., Weiss, M., Nagel, R.N. and Odrey, N.G.: Industrial robotics: Technology, programming, and applications. New York: McGraw-Hill (1986)
36. Derrac, J., García, S., Molina, D. and Herrera, F.: A practical tutorial on the use of nonparametric statistical tests as a methodology for comparing evolutionary and swarm intelligence algorithms. Swarm and Evolutionary Computation. 1(1), 3-18 (2011)

Table 1. Specification of Kawasaki RS06L robot

Specification	Value	Units
No of degrees of freedom	6	
Maximum reach	1960	mm
Work envelope	θ_1: ±180 , θ_2: +145-(-105). θ_3: +150-(-163), θ_4: ±270. θ_5: ±145, θ_6: ±360	Degrees
Configuration	All axis are completely independent and are controlled simultaneously	

Table 2. Link parameters of Kawasaki RS06L robot

Joint i	α_{i-1}	a_{i-1}	d_i	θ_i	Parameter value
1	0	0	0	θ_1	d_1=430 mm
2	90	0	0	θ_2	a_2=650mm
3	0	a_2	0	θ_3	
4	-90	0	d_4	θ_4	d_4=900mm
5	90	0	0	θ_5	
6	90	0	0	θ_6	

Table 3. Tuning parameters values of different optimization algorithms

Algori -thms	Itera-tion	Popu-lation size	Ub and Lb of design variable	γ	β	β_0	α	δ	α-damp	p_a	w	w-damp	C_1	C_2
CS	500	25	Same for all as given in Table 2	**	1.5	**	**	**	**	0.25	*	*	**	**
BA				**	**	**	**	**	**	**	*	**	**	**
HCB				**	1.5	**	**	**	**	0.25	*	*	**	**
FA				0.8	**	0.2	0.2	0.9	0.997	**	*	**	**	**
ABC				**	**	**	**	**	**	**	*	**	**	**
PSO				**	**	**	**	**	**	**	1	.99	1.5	2
TLBO				**	**	**	**	**	**	**	*	**	**	**

The '**' symbols indicates that the parameters is not a tuning parameters of that algorithm.

Table 4. Result of the Friedman ANOVA test

Algorithm Combination	p-value	Algorithm Combination	p-value
CS-BA	0.00157	HCB-PSO	0.00157
CS-HCB	0.2059	HCB-TLBO	0.52709
CS-FA	0.05778	PSO-TLBO	0.00157
CS-ABC	0.00157	TLBO-ABC	0.00157
CS-PSO	0.00157	TLBO-BA	0.00157
CS-TLBO	1	FA-ABC	0.01141
HCB-BA	0.00157	ABC-PSO	0.05778
HCB-FA	0.05778	PSO-FA	0.2059
HCB-ABC	0.00157		

Table 5. Friedman rank test result of mean error fitness value for the implemented algorithms

Algorithms	Rank	Mean Rank	Friedman Rank
CS	3	2.4	24
BA	7	6.2	62
HCB	1	1.9	19
FA	4	4	40
ABC	6	6	60
PSO	5	5.2	52
TLBO	2	2.3	23

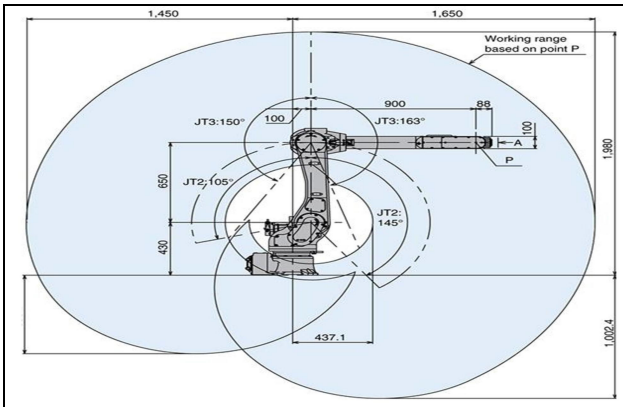

Figure 1 Kinematic model of RS06L [Kawasaki Robotics Pvt. Ltd.]

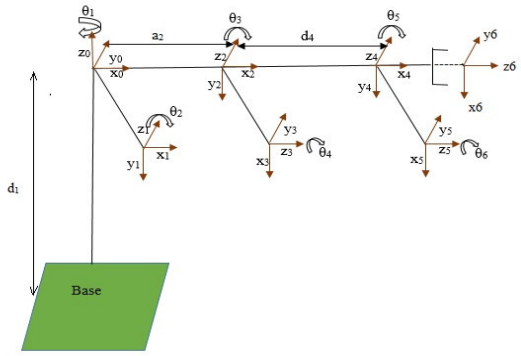

Figure 2 Schematic link diagram of the robot Kawasaki RS06L

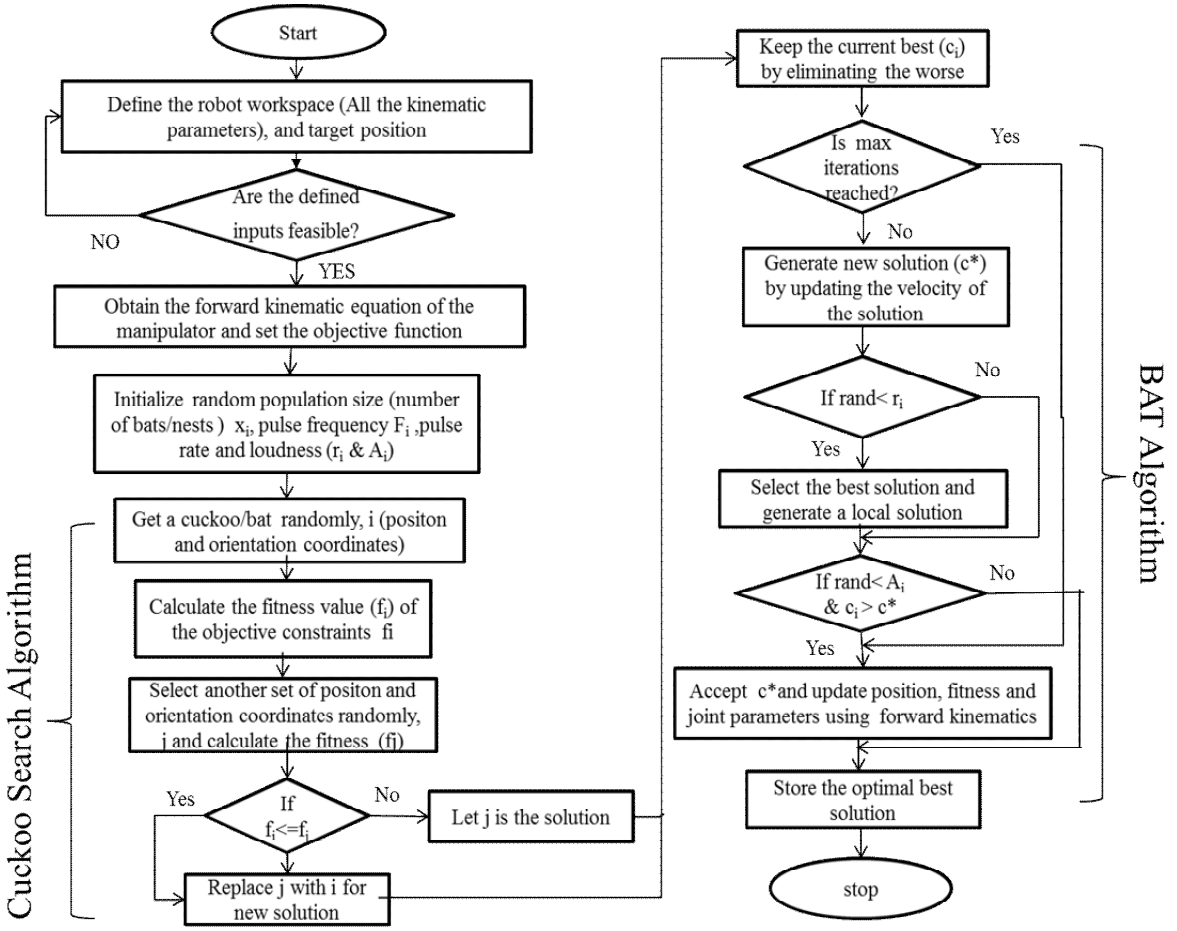

Figure 3. A flowchart for the optimal trajectory planning using the HCB scheme

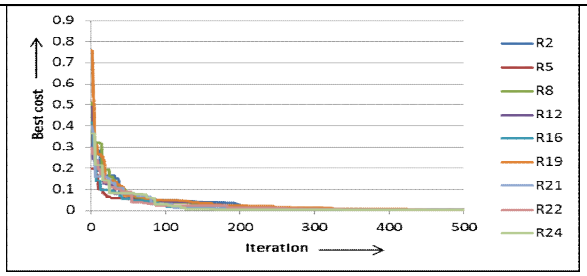

Figure 4. Convergence of HCB at different runs

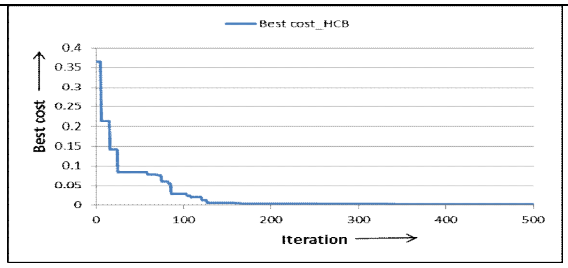

Figure 5. Best cost plot with iteration obtained from HCB

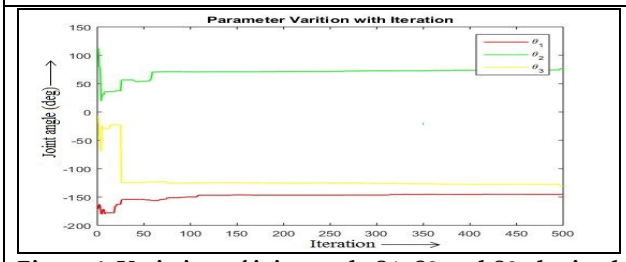

Figure 6. Variation of joint angle θ1, θ2 and θ3 obtained from HCB

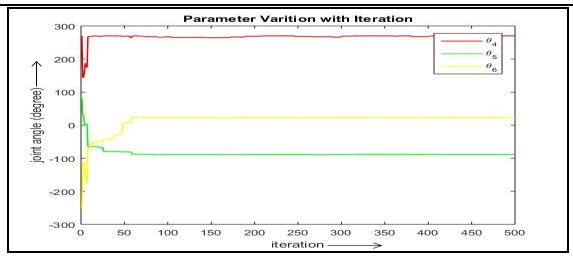

Figure 7. Variation of joint angle θ4, θ4 and θ6 obtained from HCB

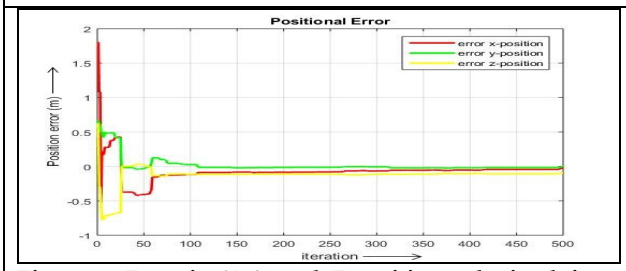

Figure 8. Error in X, Y and Z-positions obtained from HCB

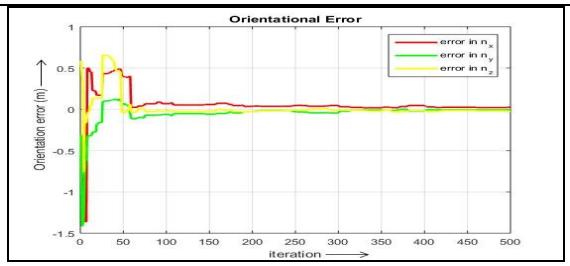

Figure 9. Error in X, Y and Z-orientation value obtained from HCB

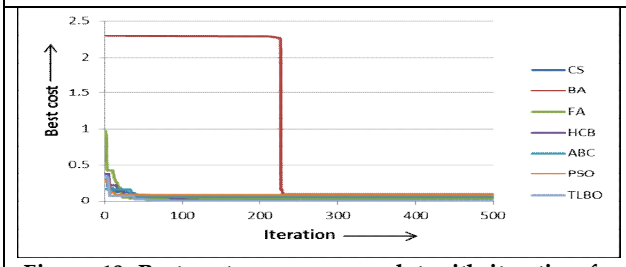

Figure 10. Best cost convergence plot with iteration for all algorithms

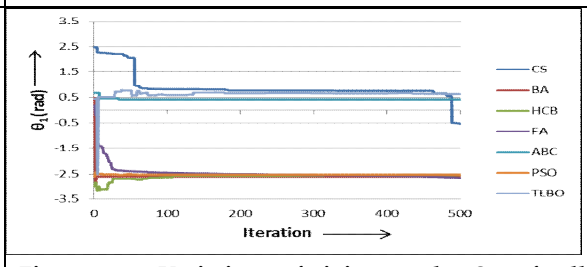

Figure 11. Variation of joint angle θ1 of all algorithms

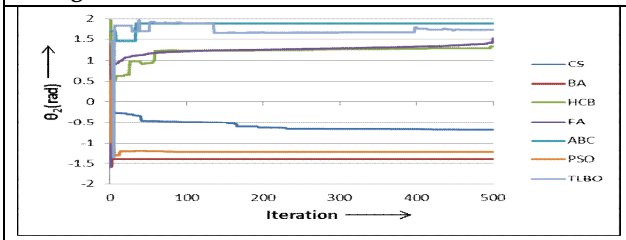

Figure 12. Variation of joint angle θ2 of all algorithms

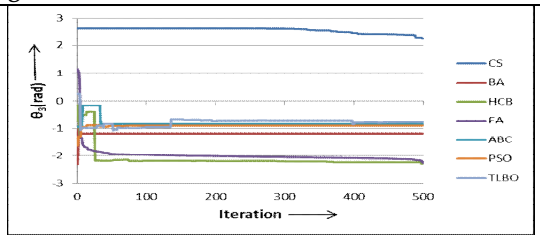

Figure 13. Variation of joint angle θ3 of all algorithms

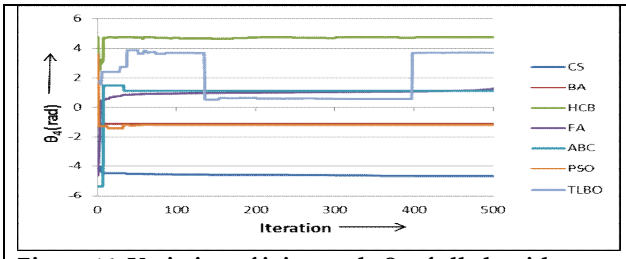

Figure 14. Variation of joint angle θ4 of all algorithms

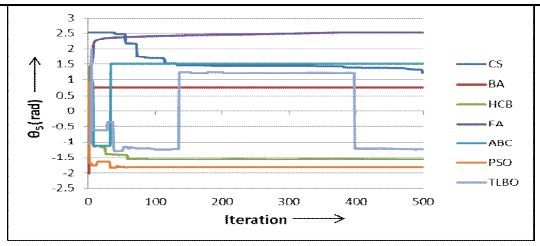

Figure 15. Variation of joint angle θ5 of all algorithms

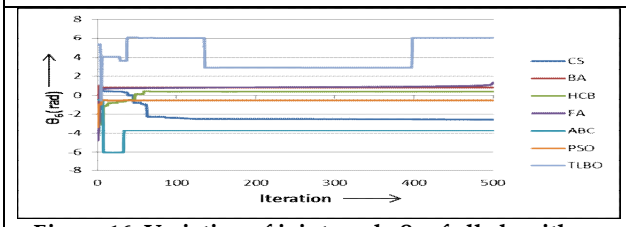

Figure 16. Variation of joint angle θ6 of all algorithms

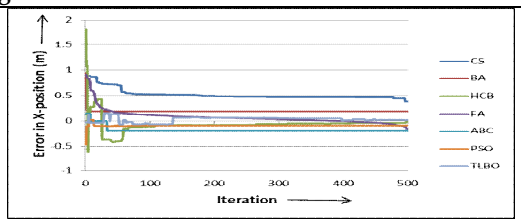

Figure 17. Error in X-positions of all algorithms

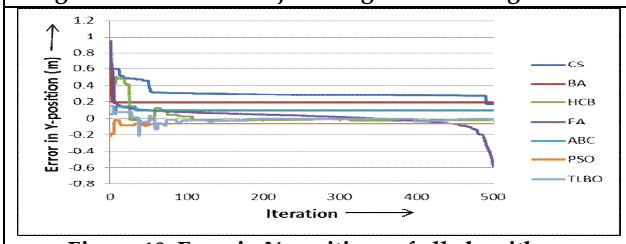

Figure 18. Error in Y-positions of all algorithms

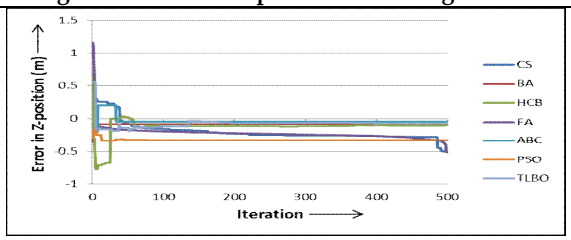

Figure 19. Error in Z-positions of all algorithms

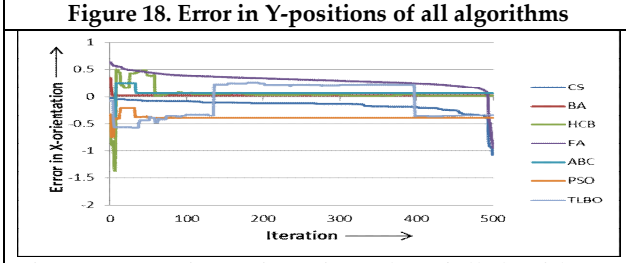

Figure 20. Error in X-orientation value of all algorithms

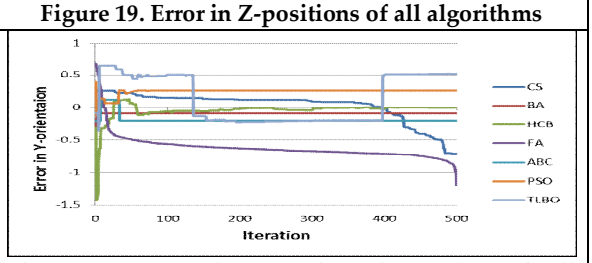

Figure 21. Error in Y- orientation value of all algorithms

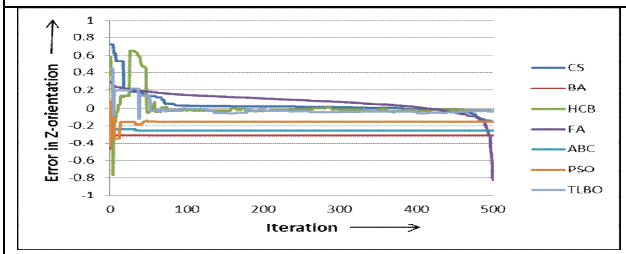

Figure 22. Error in Z- orientation value of all algorithms

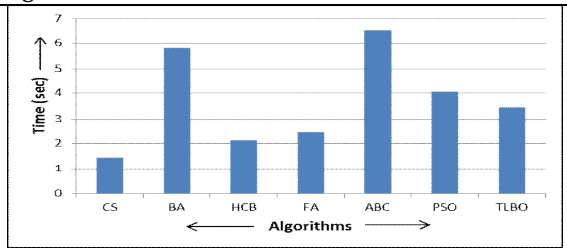

Figure 23. Computational time taken for execution of all algorithms

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RESEARCH ARTICLE

Development, Characterization and Erosive Behavior of Jute-Epoxy-TiC Hybrid Composite

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ABSTRACT

India is the largest producer of Jute in all over the world. Traditionally jute has been utilized as packaging material and decorative purpose. But in the present scenario it has been utilized in the composite industry. The most important thing is that it is a Natural fibber hence it is biodegradable. The performance of the fiber is very effective as compared to traditional artificial fiber. Light weight composite material can be prepared by using the jute fiber. It can be used in the field of automobile, Aerospace, construction and Defense Technology. This research outlines the manufacturing and mechanical description of a modern type of multi-phase composite developed from epoxy, jute fiber and titanium carbide (TiC) particles. The impact of fillers have been observed to change the physical and mechanical properties of jute epoxy composite.

Keywords: Composite, Hand Lay-up Process, Mechanical Testing, Scanning Electron Microscope

INTRODUCTION

Composite materials do provide capacity for part integration. Composites are common both in surroundings as well as among engineering materials. The components were usually macroscopic in the initial days of new man-made composite materials. As composite technology has progressed in recent decades, the component sizes, especially reinforcing materials, has been steadily decreasing. Composites are processed in four simple steps: Impregnation, lay-up, consolidation, and solidification.

MATERIAL, EQUIPMENT AND METHODS

Table 1 Material and Equipment

Matrix Material	Resin, Epoxy Araldite AW 106
Fiber Material	Jute
Particulate Filler Material	Titanium carbide (TiC)
Micro-Hardness	Leitz Micro-Hardness Tester
Universal Testing Machine	Instron 1195

Table 2 Different Composites with Compositions

Composites	Jute Fibre %wt in Epoxy	TiC % wt in Epoxy
C1	20	0
C2	30	0
C3	40	0
C4	40	10
C5	40	20

Table 3 Densities- Measured and Theoretical

Composites	Measured Density (gm/cc)	Theoretical Density (gm/cc)	Volume Fraction of Voids (%)
C1	1.127	1.135	0.71
C2	1.139	1.153	1.35
C3	1.157	1.172	1.28
C4	1.199	1.258	4.68
C5	1.287	1.358	5.22

Experimental Details

Table 4. Various Mechanical Properties

Composites	Mean Hardness (Hv)	Tensile Strength (MPa)	Flexural Strength (MPa)	Inter-laminar Shear Strength (MPa)
C1	57	302.8	312.6	20.52
C2	59	331.5	345.8	19.32
C3	63	349.6	368.6	18.42
C4	83	304.5	357.8	22.57
C5	86	279.4	353.2	28.99

Table 5. Impact Test Values

Specimen	C1	C2	C3	C4	C5
Impact test Value in Izod (No of Divisions)	23	32	41	40	38
Strength in joule. 1 div = 2 joule	46	64	82	80	76

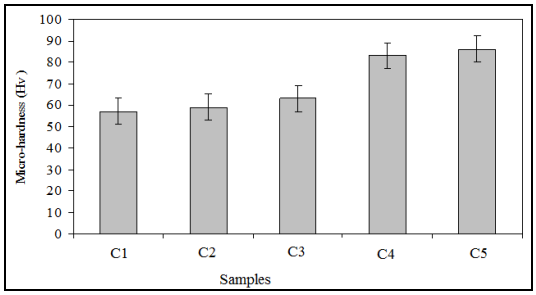

Figure. 1 Micro-Hardness Values

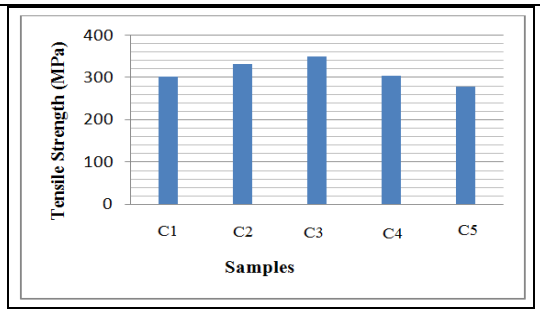

Figure. 2 Tensile Strength Values

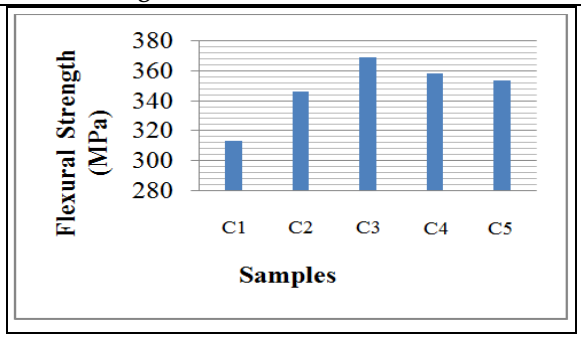

Figure 3 Flexural Strength Values

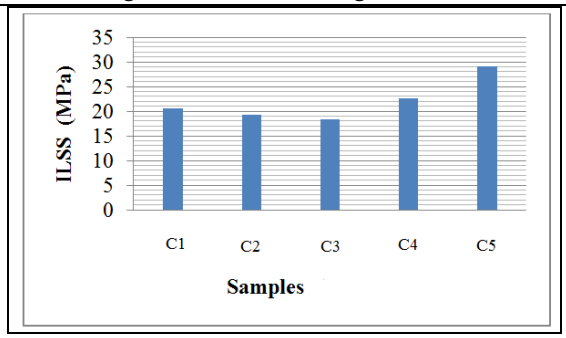

Figure.4 Inter-laminar Shear Strengths

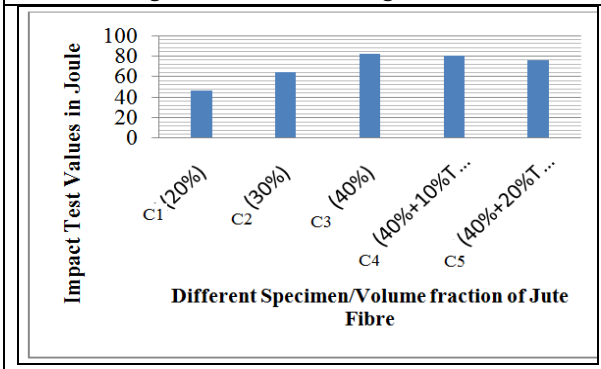

Figure 5 Comparison of Toughness

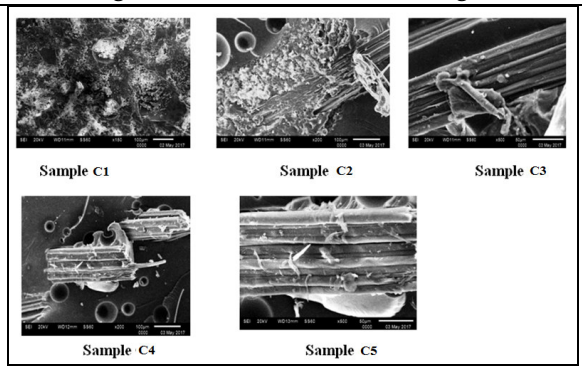

Figure 6 SEM Images after Tensile Tests

CONCLUSION

The following conclusions have been drawn from the study of the jute epoxy composite:

1. The hand lay-up method was used to effectively assemble the bidirectional jute fibre-reinforced epoxy resin.
2. The void content decreases as fiber loading increases but the hardness, tensile strength and impact strength increases.
3. Void content influences flexural strength and inter-laminar shear strength dramatically.
4. Filler content strongly affects density and hence micro-hardness.

REFERENCES

1. B. D. Agarwal and L.J. Broutman, (1990), "Analysis and performance of fiber composites", Second edition, John wiley & Sons, Inc, pp.2-16.
2. B.Z. Jang, (1994), "Advanced Polymer composites: principles and applications", ASM International.
3. J. Kuljanin, M. Vuckovic, (2002), "Influence of CdS-filler on the thermal properties of polystyrene", European Polymer Journal, 38(8):1659–1662.
4. B. Weidenfeller, M. Höfer, F. Schilling, (2004),"Thermal conductivity, thermal diffusivity, and specific heat capacity of particle filled polypropylene, Composites Part A: Applied Science and Manufacturing", 35 (4):423–429
5. T.A Stolarski, (1990), "Tribology in Machine Design", Heiman Newnes, UK.
6. K.G Budinski, (1998), "Surface Engg. for Wear Resistance", N.J, USA.
7. E. Robinowicz, (1965), "Friction and wear of materials", Willey, NY, USA.
8. H. K Thomas, (1992), "ASM Handbook: Friction, Lubrication, and Wear Technology", ASM International Handbook Committee. 18, 371-372.

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RESEARCH ARTICLE

3D Printer- Development and Printing

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ABSTRACT

The laser printer is as common as the computer system. Can't say the same about the 3D printer. But it might be about to change. 3D Printers create parts through the addition of materials and are the new hotness in the field manufacturing. Molten Polymer Deposition (MPD) or Fused Deposition Modeling (FDM) or Fused Filament Fabrication (FFF) is technique in additive manufacturing, which describes pushing a solid plastic filament into a hot-end, which then extrudes a thin stream of molten material into layers to build up the desired piece. The developed machine is used to print PLA, ABS, TPU plastics with simple design, reduced cost, maximum capacity, and increased accuracy. Simply, the heated bed makes a difference.

Keywords: 3D Printing, Hardware, Software, Materials

INTRODUCTION

You can print anything with length, width and height by a 3D printer. Plastic requires a significant melting temperature and is therefore a favorite material for three-dimensional printing. A 3D printer requires a plastic heating system before the material transforms from solid to liquid form. The hot end is heat up with electricity to melt the plastic. The extruder pushes the plastic into hot end. Motors controlled by computer and controller in a 3D printer are used for movement, spinning at varying speeds (clockwise and anticlockwise). The hot-end acts like a pen, drawing a path on the flat work surface. We have to connect 3D printer to a computer running relevant software. The software is used to build the required object and to send data to the 3D printer as instructions. If you get the hang of 3D printing, there are plenty of possibilities. The main objective was to develop a cost effective 3D printer.

Parts and Details

The 3D printer consists of parts like frame, extruder, part plate, stepper motor, circuit board, power supply, nozzle, belt, Lead Screw, Passive Block, Hand Twist Levelling Nut, Flexible Heater, Filament Sensor, Power supply cable, Lead Screw Holder (coupler), Filament, Nut and bolts, End Stop, 3D Innovation Pulley Wheel, Gantry Plate Set. It has resume printing features with v-slot linear bearing system and wheel moving parts.

CONCLUSION

a) The printer does a fantastic job printed at a much finer point 1 mm layer height the level of details is breathtaking. It makes everything take way longer to print but it almost makes the layer lines completely invisible for naked eyes.
b) Everything is attached to the frame so its nice and compact but more importantly it encapsulated the power supply so there is no exposed mains voltage unless you open it, so its relatively safe. The power supply is 24 Volts. The heated bed will heat up significantly faster and just based on results it will reach a maximum temperature of around 110 degrees Celcius
c) Though it's quite a bit smaller in size, the boat in setup is that you can print faster. If the speed is increased to 120 mm/sec, the print is also pretty cool.
d) The building volume is more than enough and which it keeps it nice and compact. It's not particularly noisy in fact it is more quiet as it has motor dampeners.
e) Flexible filament by far the most exciting filament. Through the printer flexible filaments can be printed. Bowden extruder and the extruder motor that pushes the film in forward connected by a tube to the heating element where the plastic actually gets melted that tube causes friction and is an indication to how well a 3D printer will be able to print flexible filament. In this printer the tube is small so it can print flexible filament better.

REFERENCES

1. M. Yampolskiy, A. Skjellum, M. Kretzschmar, R. A. Overfelt, K. R. Sloan, and A. Yasinsac, 2016, "Using 3D printers as weapons", Int. J. Crit. Infrastruct. Prot., vol. 14, pp. 58–71.
2. P. Minetola, M. Galati, "Challenge for enhancing the dimensional accuracy of a low-cost 3D printer by means of self-replicated parts", Additive Manufacturing.
3. B, Tymrak, M. Kreiger, J. Pearce, 2014, "Mechanical properties of components fabricated with open-source 3-D printers under realistic environmental Conditions", pp:242-6.
4. Ramya, S.L. Vanapalli, 2016,"3D Printing Technologies in various applications", International Journal of Mechanical Engineering and Technology (IJMET), 7(3): 396-409.
5. T. Femmer, A. J. C. Kuehne, and M. Wessling, 2015, "Estimation of the structure dependent performance of 3-D rapid prototyped membranes", Chem. Eng. J., vol. 273, pp. 438–445.

Table 1 Important Parts

Printer Controller Board	RAMPS 1.4 3D Printer controller+Mega2560 with cable +5Pcs A4988 Driver with Heat Sink Kit; Fits 5 Pololu stepper driver board.
Stepper Motor	Bipolar Nema 17
Hardware	Smooth and threaded rods; Linear bearing , ball bearing , coupling , belt , GT pulley , GT 2 belt; Aluminium Frame
Hot End	Magma Hot end kit (Thermister& resistor included) 40 mm Fan & its Holder.

Table 2.2 Printer Description

Modeling Technology	Fluid Deposition Modeling
Printing Size	220 mm x 220mm x 250 mm
Printing Accuracy	0.1 mm
Max. Travelling Speed	180 mm/sec
Filament	Diameter- 1.75 mm
Layer Thickness	0.1 mm-0.3 mm
Nozzle Diameter	0.4 mm
Extruder	Mk-10
File Format	.stl
Software	Ultimaker Cura
Maximum Nozzle Temperature	225 Degree Celcius
Hotbed Temperature	110 Degree Celcius

CATIA Design

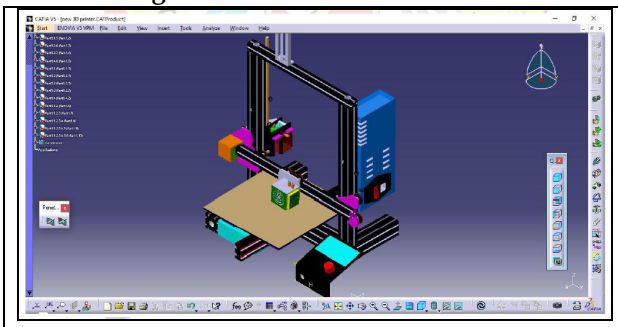

Figure .1 Isometric View- 3D Printer

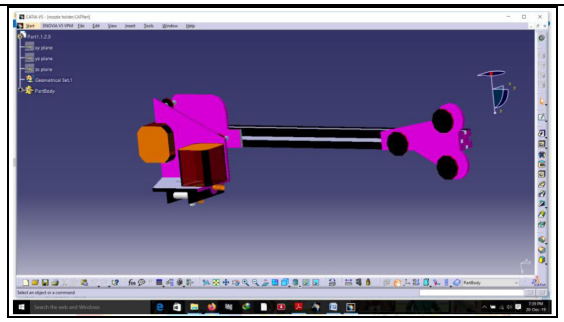

Figure .2 Extruder Holder and Frame

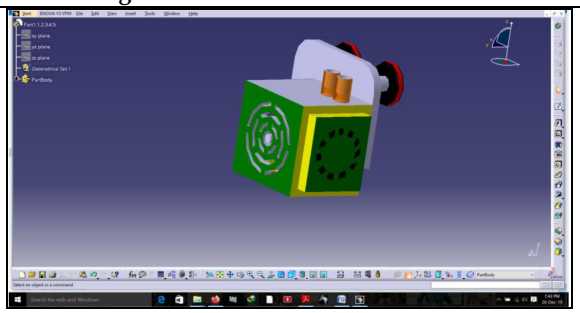

Figure .3 Extruder

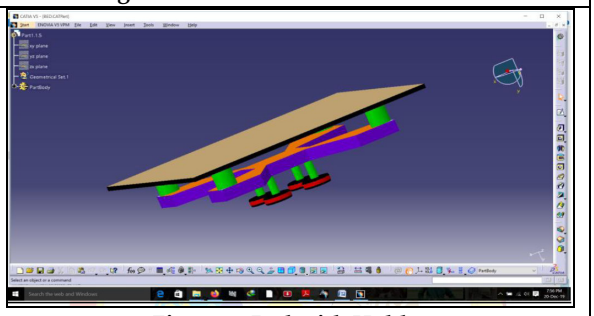

Figure .4 Bed with Holder

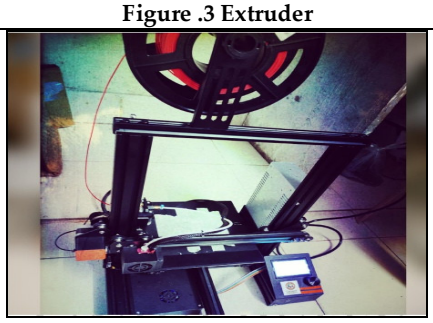

Figure .5 3D Printer

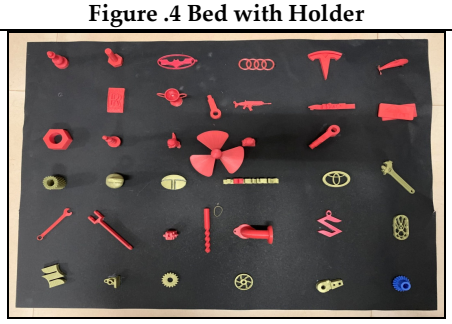

Figure .6 Printed Products

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RESEARCH ARTICLE

Performance Analysis of EDM Process Using Different Tools

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ABSTRACT

The present study is carried out to assess the best combination of process parameters which will satisfy multiple objectives like lesser tool wear, greater material removal and lower surface roughness value in Electric Discharge Machining (EDM) of D2 Steel by varying the tool. Direct metal laser sintered electrode using Directmetal20 has been selected along with traditionally used electrodes like copper and brass to assess the possibility of replacing these traditional electrodes by DMLS electrode. The study makes use of Grey relational analysis along with the Taguchi method to develop a hybrid method which can solve multi-objective optimization problems unlike the traditional Taguchi method. Confirmatory test is performed to validate the effectiveness of the method.

Keywords: Multi-objective optimization; grey relational analysis; Taguchi method; electric discharge machining, direct metal laser sintering

INTRODUCTION

EDM is a highly developed non-traditional machining process which is employed to machine any electrically conductive metal by using thermal energy. It is capable of producing any complex shape and size. Due to this it finds extensive application in the manufacturing of automobile and aerospace components of complex shape and size. EDM is performed with a system involving a machine tool and a power supply. A sequence of spark produced between the tool and work causes material removal from the work. The common performance measures in any machining (both traditional and non-traditional) are material removal rate (MRR), tool wear rate (TWR) and surface roughness (R_a) of the generated cavity. The EDM tool has maximum influence on these performance parameters.

Simultaneous optimization of these performance measures by considering different EDM tools as a process variable can further help in the development in EDM.

Literature study and objective of the research

Complexity of eroded cavity increases the cost of EDM machining. In order to minimize the cost of production of EDM tool and time for product development different innovative methods to produce EDM tool have been explored. Rapid prototyping (RP) technology refers to a group of advanced and innovative manufacturing methods where the parts are created by addition of materials on layer-by-layer basis. A good number of researchers have taken the help of different RP technologies to create EDM tools. Arthur et al. [1] engaged thin coated Stereo Lithography (SL) models to machine hardened tool steel. Those electrodes found their suitability for semi-roughing as well as finishing operations in EDM. Rennie et al. [2] created complex EDM electrodes by applying electroforming to rapid prototyping which offered performance comparable with the traditional solid copper electrode. Durr et al. [3] used direct metal laser sintering (DMLS) to manufacture simple cylindrical metal electrodes using metal powders of bronze, nickel and copper phosphite. Greater tool wear and worse surface quality was observed in comparison with conventional electrodes. Dimla et al. [4] produced intricate components having sloped surfaces and deep slots by electroplating of DMLS electrodes.

Meena and Nagahanumaiah [5] studied the influence of EDM process parameters on workpiece with DMLS electrodes. The wear at the front edge of the electrode was found to be greater than wear at the side as a result of the porosity of the DMLS electrodes. Czyzewski et al. [6] manufactured EDM electrodes by 3D printing technology. Amorim et al. [7] used tools made by selective laser sintering (SLS) using different powder materials. Ferraris et al. [8] examined the behavior of ceramic composites in EDM and studied their impact on MRR, relative tool wear and R_a. Czelusniak et al. [9] focused on the choice of suitable ingredients to produce EDM electrode using selective laser sintering. They performed experiments by varying discharge energies and calculated the MRR and volumetric relative wear (VRW). Mohanty et al. [10] also performed EDM operation with electrodes prepared by DMLS using Directmetal 20 and found peak current to be the most important factor followed by spark-on time. Reddy et al. [11] manufactured EDM electrodes by electroless coating of parts made up of PLA and ABS materials produced by fused deposition modelling.

The electrical conductivity of PLA based electrode was found to be more than the conductivity of ABS based electrode. Padhi et al. [12] found the suitability of thick copper-electroplated FDM ABS plastic electrode for rough cutting and semi-finishing operation of D2 steelIn this case due to inability of conventional Taguchi technique to address problems with multiple objectives, grey relational analysis has been combined with Taguchi method. This method known as grey Taguchi method [13] is one of the many hybrid Taguchi methods used in solving multi response optimizations. Other well-known hybrid Taguchi methods are principal component based Taguchi method [14], utility concept based Taguchi method [15] and desirability concept based Taguchi method [16] etc. Grey Taguchi method is chosen because it requires less mathematical calculations compared to the other hybrid Taguchi methods. Detailed method has been explained in this paper.

Taguchi method

Taguchi method is a state-of-the-art method to resolve single objective optimization problems with minimum number of experiments. It uses Signal-to-Noise (S/N) ratio [17] as a measure of performance. The S/N ratio rests on the quality characteristics of the process. The S/N ratios for three possible situations used are presented by Eqs. (1-3).The best setting corresponds to the maximum S/N ratio.

Higher-the-better (HB)

$$\text{S/N ratio} = -10\log_{10}\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{y_i^2}\right) \quad (1)$$

Here, *n* represents number of repetitions and y_i is the measured output. This is used where higher value is required such as agricultural yield, petrol mileage, or tensile strength of a material.

Lower-the-better (LB)

$$\text{S/N ratio} = -10\log_{10}\left(\frac{1}{n}\sum_{i=1}^{n} y_i^2\right) \quad (2)$$

Here, *n* represents number of repetitions and y_i is the measured output. This is used where lower value is required such as emission of a vehicle and corrosion in metal surface etc.

Nominal-the-best (NB)

$$\text{S/N ratio} = -10\log_{10}\left(\frac{\mu^2}{\sigma^2}\right) \quad (3)$$

Here, μ = mean and σ = Standard deviation. This is used where attaining a nominal or target value is required such as diameter of spindle to be attained and weight of product to be maintained etc.

Grey relational analysis (GRA) based Taguchi Method

Grey relational analysis helps in converting problem with more than one objective into problem with a single objective which can then be solved by Taguchi method.

In the first step of the grey relational analysis, measured values of the responses are normalized in the range between 0 and 1. The normalized data for smaller-the-better condition is represented as:

$$a_i(\mathrm{k}) = \frac{\max b_i(\mathrm{k}) - b_i(\mathrm{k})}{\max b_i(\mathrm{k}) - \min b_i(\mathrm{k})} \quad (4)$$

The normalized data for larger-the-better condition is represented as,

$$a_i(\mathrm{k}) = \frac{b_i(\mathrm{k}) - \min b_i(\mathrm{k})}{\max b_i(\mathrm{k}) - \min b_i(\mathrm{k})} \quad (5)$$

where $a_i(\mathrm{k})$ is the normalized value, $\min b_i(\mathrm{k})$ is the smallest value of $b_i(\mathrm{k})$ for the k^{th}response and $\max b_i(\mathrm{k})$ is the largest value of $b_i(\mathrm{k})$ for the k^{th} response. An ideal sequence is $a_0(\mathrm{k})$ for the responses.

In the second step grey relational numbers are computed on the basis of the normalized data. The grey relational number $\xi_i(\mathrm{k})$ is given as

$$\xi_i(\mathrm{k}) = \frac{\Delta_{\min} + \psi\Delta_{\max}}{\Delta_{0i}(\mathrm{k}) + \psi\Delta_{\max}} \quad (6)$$

Here $\Delta_{0i} = \|a_0(\mathrm{k}) - a_i(\mathrm{k})\|$ = difference of the absolute value $a_0(\mathrm{k})$ and $a_i(\mathrm{k})$; ψ is the differentiating coefficient $0 \le \psi \le 1$; $\Delta_{\min} = \forall j^{\min} \in i \forall k^{\min} \|a_0(\mathrm{k}) - aj(k)\|$ = the smallest value of Δ_{0i}; and $\Delta_{\max} = \forall j^{\max} \in i \forall k^{\max} \|a_0(\mathrm{k}) - aj(k)\|$ = largest value of Δ_{0i}.

In the third step the overall grey relational score (OGRS) which is denoted by γ_i is calculated. γ_i is the mean of the grey relational numbers and is given as:

$$\gamma_i = \frac{1}{n}\sum_{k=1}^{n}\xi_i(\mathrm{k}) \tag{7}$$

n represents total number of outputs(responses). The greater value of grey relational score indicates to intense relational degree between $a_0(\mathrm{k})$ and $a_i(\mathrm{k})$. Therefore, higher grey relational score indicates better quality.
By taking this OGRS as a single objective, the problem is solved by traditional Taguchi method.

Experimentation
The process parameters selected are peak current (I_P), spark-on time (T_{on}), spark-off time (T_{off}), flushing pressure (F_P) and tool electrode (TE). TWR, MRR and R_a have been selected as response variables. D2 steel has been selected as work piece. Different process parameters along their levels during EDM are given in Table 1. Three cylindrical tools (20mm x 20mm) selected were brass, copper and DMLS part. DMLS is a developed RP process to form 3D parts. DMLS part has been prepared employing EOSINT M250 Extended machine using DirectMetal20 as a powder material. The schematic diagram of the direct metal laser sintering process is shown in Fig 1. Computer aided design (CAD) model (in .STL format) was sliced by means of "EOS RP Tools" and transmitted to the process compute. PSW software was used to create the laser path. Laser power, layer thickness, hatch width, hatch spacing and laser scan speed during the sintering process have been kept at 228W, 40µm, 5mm, 0.2mmand 500mm/sec respectively. Sintering was carried out in nitrogen environment (with O_2 < 1.5%). Wire EDM was used to remove the platform from the base plate.

RESULTS AND ANALYSIS

The results of the experiments performed following Taguchi's L27 OA design have been presented in Table 2. The normalized experimental data using Eqs.(4) and (5) are shown in Table 3. SB criteria are used for TWR & R_a, while a LB criterion is used for MRR. Quality loss estimations (Δ_{0i}) associated with the individual quality characteristics are provided in Table 4. Then grey relational numbers for individual quality characteristics are computed using Eq. (6) and are presented in Table 5. The distinguishing coefficient (Φ) is taken as 0.5. The overall grey relational score is calculated using Eq. (7), which represents the multi-quality features. The evaluated OGRS values are presented in Table 5. The predicted ideal setting for optimum OGRS using Taguchi method becomes $I_{p1}T_{on3}T_{off3}F_{p1}TE_1$ (observed from main effects plot for S/N ratio presented in Fig. 2). Then a confirmatory test has been performed to validate the predicted settings. R-Sq value of 92.66% indicates the effectiveness of carrying out the tests. The ANOVA for OGRS presented in Table 6 indicates tool electrode (TE) to be the most important factor. OGRS is in decreasing order for brass, copper and DMLS electrodes.

CONCLUSIONS

The following observations have been made from the results of the experiments:
1) Best parametric combination can be found out by combining GRA with Taguchi method.
2) Confirmatory test has been done to endorse the predicted best setting $(I_{p1}T_{on3}T_{off3}F_{p1}TE_1)$ obtained.
3) TE is found to be the most important factor affecting the output.
4) This cited technique can be suggested for solving other similar problems.

5) The DMLS electrode has offered inferior performance compared to both the conventional electrodes (brass and copper) used in the study. The poor performance of DMLS electrode is owing to the higher porosity level. So porosity level of DMLS electrode should be significantly reduced to make it suitable as a substitute for conventional electrodes like copper and brass.
6) DMLS electrode may be recommended for roughing and semi-finishing operation.

REFERENCES

1. Arthur A, Dickens P M and Cobb R C 1996 Using rapid prototyping to produce electrical discharge machining electrodes, *Rapid Proto. J*. 2(1): 4–12.
2. Rennie A E W, Bocking C E and Bennett G R 2001 Electroforming of rapid prototyping mandrels for electro-discharge machining electrodes, *J. Mater. Process Tech*. 110: 186–196.
3. Durr H, Pilz R and Eleser N S 1999 Rapid tooling of EDM electrodes by means of selective laser sintering, *Comput. Ind*. 39: 35–45.
4. Dimla D E, Hopkinson N and Rothe H 2004 Investigation of complex rapid EDM electrodes for rapid tooling applications, *Int. J. Adv. Manuf. Technol*. 23: 249–255.
5. Meena V K and Nagahanumaiah 2006 Optimization of EDM machining parameters using DMLS electrode, *Rapid Proto. J*, 12(4), (2006), pp.222-228.
6. Czyzewski J, Burzynski P, Gaweł K and Meisner, J 2009 Rapid prototyping of electrically conductive components using 3D printing technology, *J. Mater. Process. Technol*. 209: 5281–5285.
7. Amarim F L, Lohrengel A, Miller N, Schafer G and Czelusniak T 2013 Performance of sinking EDM electrodes made by selective laser sintering technique, *Int. J. Adv. Manuf. Technol*. 65: 1423-1428.
8. Ferraris, E., Reynearts, D. and Lauwers, B. (2011) Micro-EDM process investigation and comparison performance of Al3O2 and ZrO2 based ceramic composites. CIRP Annals - Manufacturing Technology 60(1): 235–238.
9. Czelusniak, T L, Amorim, F L, Higa, C F and Lohrengel, A. (2014) Development and application of new composite materials as EDM electrodes manufactured via selective laser sintering. *Int. J. Adv. Manuf. Technol*, 72: 1503-1512.
10. Mohanty S D, Mahapatra S S and Mohanty R C 2017 Study on performance of EDM electrodes produced through rapid tooling route. J. Adv. Man. Sys. 16 (4): 357-374.
11. Reddy L M, Krishna L S R, Kumar S S and Reddy P R (June 2018) Estimation of electrical conductivity of ABS and PLA based EDM electrode fabricated by using FDM 3D-Printing process. *Int. J. Mod. Eng. Res. Technol*.5: 332-338.
12. Padhi S K, Mahapatra S S, Padhi R, Das H C (December 2018) Performance analysis of a thick copper-electroplated FDM ABS plastic rapid tool EDM electrode. Adv. Manuf.6(4): 442-456.
13. Datta, S.; Bandyopadhyay, A.; Pal, P.K.: Grey based Taguchi method for optimization of bead geometry in submerged arc bead-on-plate welding. Int. J. Adv. Manuf. Technol. 39, 1136-1143 (2008)
14. Routara, B.C.; Mohanty. S.D.; Datta, S.; Bandyopadhyay, A.; Mahapatra, S.S.: Combined quality loss (CQL) concept in WPCA-based Taguchi philosophy for optimization of multiple surface quality characteristics of UNS C34000 brass in cylindrical grinding.Int. J. Adv. Manuf. Technol. 51(1), 135-143 (2010)
15. Kumar, P.;Barua, P.B.; Gaindhar, J.L.: Quality optimization (multi-characteristics) through Taguchi's technique and utility concept. Quality and Reliability Engg Int. 16, 475-485 (2000)
16. Datta, S.; Bandyopadhyay, A.; Pal, P.K.: Desirability function approach for solving multi-objective optimization problem in submerged arc welding. Int. J. Manuf. Science and Prod. 7(2), 127-135 (2006)
17. Zhao, J.; Li, Y.; Zhang, J.; Yu, C.; Zhang, Y.: Analysis of the wear characteristics of an EDM electrode made by selective laser sintering. J. Mater Process Technol. 138, 475–478 (2003)

Table 1: Process parameters along with their levels

Levels	I_p (A)	T_{on} (µs)	T_{off}(µs)	F_p (kN/m²)	*TE*
1	7.5	120	10	30	Brass
2	10	150	20	60	Copper
3	12.5	180	30	90	DMLS

Table 2 Experimental results along with design matrix

Sl. No.	L27 OA					Measured responses		
	I	T_{on}	T_{off}	F_p	Tool	TWR	MRR	R_a
1	1	1	1	1	1	10.379	9.286	2.108
2	1	1	1	1	2	5.425	9.895	2.938
3	1	1	1	1	3	6.69	5.991	3.698
4	1	2	2	2	1	8.361	12.982	1.925
5	1	2	2	2	2	5.145	13.145	3.028
6	1	2	2	2	3	7.581	6.77	4.365
7	1	3	3	3	1	7.415	11.995	1.898
8	1	3	3	3	2	4.025	12.045	2.665
9	1	3	3	3	3	6.028	6.873	3.138
10	2	1	2	3	1	7.735	12.688	2.281
11	2	1	2	3	2	5.345	12.982	3.571
12	2	1	2	3	3	4.604	2.429	4.788
13	2	2	3	1	1	9.252	17.208	2.345
14	2	2	3	1	2	5.365	17.783	3.345
15	2	2	3	1	3	5.774	9.992	5.131
16	2	3	1	2	1	11.935	12.495	2.308
17	2	3	1	2	2	7.945	12.395	3.528
18	2	3	1	2	3	8.232	5.311	3.975
19	3	1	3	2	1	12.015	18.427	2.308
20	3	1	3	2	2	9.515	19.195	3.455
21	3	1	3	2	3	10.619	12.826	5.255
22	3	2	1	3	1	14.115	17.195	2.781
23	3	2	1	3	2	10.645	15.815	3.898
24	3	2	1	3	3	11.231	9.733	5.081
25	3	3	2	1	1	15.395	19.995	2.645
26	3	3	2	1	2	10.495	20.295	3.931
27	3	3	2	1	3	11.455	12.634	4.571

Table 3 Normalized experimental data

Sl. No.	Normalized value of TWR	Normalized value of MRR	Normalized value of Ra
Ideal	1	1	1
1	0.4412	0.3838	0.9374
2	0.8769	0.4179	0.6902

3	0.7656	0.1994	0.4638
4	0.6186	0.5907	0.992
5	0.9015	0.5998	0.6634
6	0.6872	0.243	0.2651
7	0.7018	0.5354	1
8	1	0.5382	0.7715
9	0.8238	0.2487	0.6306
10	0.6737	0.5742	0.8859
11	0.8839	0.5907	0.5016
12	0.9491	2.00E-17	0.1391
13	0.5403	0.8272	0.8668
14	0.8821	0.8594	0.569
15	0.8462	0.4233	0.0369
16	0.3043	0.5634	0.8779
17	0.6552	0.5578	0.5144
18	0.63	0.1613	0.3813
19	0.2973	0.8954	0.8779
20	0.5172	0.9384	0.5362
21	0.4201	0.5819	0
22	0.1126	0.8265	0.737
23	0.4178	0.7492	0.4042
24	0.3662	0.4088	0.0518
25	0	0.9832	0.7775
26	0.431	1	0.3944
27	0.3465	0.5712	0.2038

Table 4 Calculations of quality loss estimations

Sl. No.	Quality loss estimations of TWR	Quality loss estimations of MRR	Quality loss estimations of Ra
Ideal	0	0	0
1	0.5588	0.6162	0.0626
2	0.1231	0.5821	0.3098
3	0.2344	0.8006	0.5362
4	0.3814	0.4093	0.008
5	0.0985	0.4002	0.3366
6	0.3128	0.757	0.7349
7	0.2982	0.4646	0
8	0	0.4618	0.2285
9	0.1762	0.7513	0.3694
10	0.3263	0.4258	0.1141
11	0.1161	0.4093	0.4984
12	0.0509	1	0.8609
13	0.4597	0.1728	0.1332
14	0.1179	0.1406	0.431
15	0.1538	0.5767	0.9631
16	0.6957	0.4366	0.1221

17	0.3448	0.4422	0.4856
18	0.37	0.8387	0.6187
19	0.7027	0.1046	0.1221
20	0.4828	0.0616	0.4638
21	0.5799	0.4181	1
22	0.8874	0.1735	0.263
23	0.5822	0.2508	0.5958
24	0.6338	0.5912	0.9482
25	1	0.0168	0.2225
26	0.569	0	0.6056
27	0.6535	0.4288	0.7962

Table 5 Individual grey relational numbers and OGRS

Sl. No.	Grey relational numbers for TWR	Grey relational numbers for MRR	Grey relational numbers for R_a	Overall grey relational score
1	0.4722	0.4479	0.8887	0.6029
2	0.8024	0.4621	0.6174	0.6273
3	0.6808	0.3844	0.4825	0.5159
4	0.5673	0.5499	0.9843	0.7005
5	0.8354	0.5554	0.5977	0.6628
6	0.6152	0.3978	0.4049	0.4726
7	0.6264	0.5183	1	0.7149
8	1	0.5199	0.6863	0.7354
9	0.7394	0.3996	0.5751	0.5714
10	0.6051	0.5401	0.8142	0.6531
11	0.8116	0.5499	0.5008	0.6208
12	0.9076	0.3333	0.3674	0.5361
13	0.521	0.7432	0.7896	0.6846
14	0.8092	0.7805	0.5371	0.7089
15	0.7648	0.4644	0.3417	0.5236
16	0.4182	0.5338	0.8037	0.5852
17	0.5919	0.5307	0.5073	0.5433
18	0.5747	0.3735	0.4469	0.465
19	0.4157	0.827	0.8037	0.6821
20	0.5088	0.8903	0.5188	0.6393
21	0.463	0.5446	0.3333	0.447
22	0.3604	0.7424	0.6553	0.586
23	0.462	0.666	0.4563	0.5281
24	0.441	0.4582	0.3453	0.4148
25	0.3333	0.9675	0.692	0.6643
26	0.4677	1	0.4522	0.64
27	0.4335	0.5383	0.3857	0.4525

Table 6 ANOVA for OGRS

Source	DF	Seq SS	Adj SS	Adj SS	F	P
I	2	0.016786	0.016786	0.008393	8.27	0.003
T_{on}	2	0.000451	0.000451	0.000226	0.22	0.803
T_{off}	2	0.040056	0.040056	0.020028	19.73	0.000
F_p	2	0.002941	0.002941	0.001470	1.45	0.264
TE	2	0.144856	0.144856	0.072428	71.35	0.000
Error	16	0.016242	0.016242	0.001015		
Total	26	0.221333				

S = 0.0318613 R-Sq = 92.66% R-Sq (adj) = 88.08%

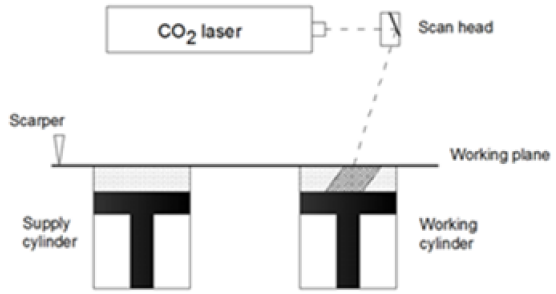

Fig.1 Schematic diagram of DMLS process

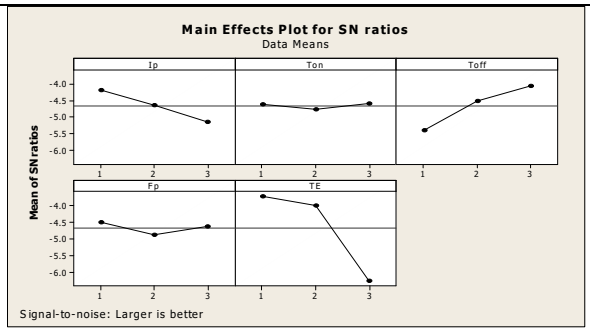

Fig. 2 Main effects plot for S/N ratio (Evaluation of optimal setting)

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RESEARCH ARTICLE

Biogas Enrichment by Water Scrubbing

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ABSTRACT

This work presents the development of biogas purification system through water scrubbing to substitute the fuels used in cooking and I.C. engine applications. A water scrubber is designed to remove carbon dioxide from raw biogas through physical absorption method by water at a pressure of 3-4 bar. It is found from the test that the scrubbing unit can remove 89.74% of carbon dioxide present in the raw biogas. After water scrubbing, cleaning of biogas is done through desulphurization to remove hydrogen sulphide and dehydration to remove moisture present in the biogas. The purified and enriched biogas is used as alternate fuel for running the I.C. engine to produce power and as cooking fuel in rural households.

Keywords: Anaerobic digestion, desulphurization, dehydration, kitchen wastes, I.C. engines, chromatography

INTRODUCTION

The continuous generation of organic wastes like municipal wastes, kitchen wastes and dairy wastes are becoming environmental and social issues for their improper treatments. It is therefore required to decompose the organic wastes to produce biogas. Anaerobic digestion is one of the processes to decompose the organic wastes into methane, carbon dioxide and other constituents in absence of oxygen. In this process microbial decomposition of organic wastes occurs which is also known as bio-methanogenesis to produce methane. Anaerobic digestion has the advantage of biogas production and contribution to the conservation of non- renewable energy sources. In this context, we have installed a small biogas plant of 2 m^3capacity to use kitchen wastes as feed stock. A water scrubbing unit has been designed and developed for biogas purification to remove carbon dioxide and cleaning to remove hydrogen sulphide and water moisture for utilization as fuel in cooking applications and as an alternate fuel for I.C. engines.

BIOGAS PURIFICATION

Application of biogas technology has already gained acceptance in developed and developing countries both at the community usage and commercial applications although on a limited scale. The biogas produced by anaerobic digestion is a clean, cheap and efficient fuel containing about 50-60% of methane (CH_4), 30-40% carbon dioxide (CO_2), 1-6% other gases and traces of hydrogen sulphide (H_2S). Carbon dioxide and hydrogen sulphide present in the biogas are insignificant for practical purposes and occupy considerable amount of volume in storage system. For better heating values in cooking and I.C. engine applications, these gases should be removed to make the biogas suitable for applications as is the case with natural gas which contains more than 90% CH_4. The biogas purification aims to increase the lower calorific value of the biogas and convert it to higher fuel standard [14]. If the biogas is purified to specifications similar to natural gas, the final gas product is called biomethane. In the upgrading process, the CO_2 contained in the raw biogas is either removed or is converted to CH_4 by reaction with H_2 [9]. In the process of water scrubbing, CO_2 has the affinity of absorption with water resulting more amount of CH_4 content in the purified biogas. Therefore, high pressure water can be sprayed on pressurized raw biogas and large amounts of CO_2 gas will be absorbed resulting more amount of CH_4 [1]. Biogas upgrading through other fermentation processes, CO_2 in biogas can be biologically converted to methane with the addition of H_2 [8].In some cases H_2S and CO_2 should be removed depending upon the specific gas utilization as shown in the table 1 [6].

SCRUBBING OF CARBON DIOXIDE

The feasible processes of removal of CO_2 from biogas are generally classified into 5 groups as follow [4, 2].

- Absorption in toliquid
- Adsorption on solid surface
- Cryogenic separation
- Chemical conversion to another compound
- Membrane separation

Absorption in to liquid

Absorption is one of the most commonly used processes for purification of biogas. In this process, gas dissolves in the liquid through phase boundary and absorption involves mass transfer in opposite direction from liquid to gas phase. Absorbers used in most gas treatment processes are either packed plate or spray towers. In general the absorber types are interchangeable to a considerable extent although certain specific conditions may favor one over the other. Absorption process can be classified in to two major groups; mainly physical absorption and chemical absorption. The major difference between physical and chemical solvents lays in their phase equilibrium characteristics with respect to carbon dioxide.

Physical absorption process

In physical absorption process water under pressure absorbs CO_2 which is called water scrubbing. It is the simplest method to remove CO_2 from biogas, but higher amount of water is required in this process. The flow diagram of water-absorption method is shown in Fig. 1 [11]. The absorption unit consists of an absorption column operating at high pressure and $CO_2$is mixed with water in theflash chamber. In water absorption method biogas is feed intothechamberatthebottomandwaterissprayedfromthetopforpropermixingofbiogaswithwater.TheCO_2contentdecreases with increase in CH_4. In thisprocesshighpressure water and high pressure biogas aresuppliedto the absorption tower[12].

WATER SCRUBBING METHODOLOGY

Biogas from kitchen wastes is a renewable source of energy for both cooking and I.C. engine applications. For larger quantities of production, it is difficult to store and transport due to high volume content of $CO_2$and H_2S in biogas. Therefore it is required for scrubbing to remove $CO_2$and H_2S. A water scrubbing method is adopted to remove $CO_2$to produce enriched biogas for cooking and I.C. engine applications.

The scrubbing unit consists of a vertical cylindrical tower with three perforated trays mounted horizontally. Biogas enters the tower at the bottom and travels upward through openings in the trays, while the water flows from the top and across each tray. The gas mixes with the water flowing over the tray, providing more gas-water contact. The gas velocity prevents water from flowing down through the perforations in the tray. The bottom end is equipped with biogas inlet and waste water outlet. The top end provides water inlet and gas outlet. After the scrubbing, the purified gas leaves the tower and passes through desulphurizer to remove H_2S and dehydrator to remove moisture. Then the enriched biogas is stored for cooking and I.C. engine applications.

Experimental design of water scrubber

A cylindrical scrubbing column of height 3000 mm and diameter 150 mm is designed and fabricated as shown in Fig. 2. The temperature range of water is 20-50^{o}C and flow rate is 2 m^3/hr at pressure of 4 bar. Inlet pressure of biogas is 3 bar and the flow rate is 1.5 m^3/hr. The raw biogas is compressed up to 8-10 bar pressure and stored in the compressor vessel. A reciprocating pump is used to supply pressurized water at 4 bar, which is used as an absorbent liquid. Perforated plates are used as packing material.

Components of water scrubbing unit

The water scrubbing unit consists of a scrubbing tower with perforated trays, a reciprocating pump to supply high pressure water, a reciprocating compressor to supply pressurized biogas, an elastic balloon to store enriched biogas, a desulphurizer to remove H_2S, a dehydrator to remove moisture, pipe fittings and different accessories like pressure gauges and regulatory valves. The complete biogas enrichment unit is shown in Fig. 3.

Scrubbing tower

The scrubbing tower consists of transparent fibre cylinders joined vertically and provided with 3 perforated trays. They are held by 3 mild steel tie rods bolted at top and bottom. The tower is supported by fabricated mild steel frame with a stand. The details of the scrubbing tower are shown in table 3. The schematic view of the scrubbing tower is shown in Fig. 4.

The scrubbing tower is divided in to three sections, as given below.

Top Section : The top section of the scrubber consists of a 5 mm thick mild steel plate provided with 15 mm purified gas outlet pipe, 15 mm water inlet pipe and 3 mm water spraying nozzle as shown in Fig. 5. The top plate is bolted with the bottom plate by means of three tie rods of diameter 10 mm. Schematic diagram of top view with dimensions is shown in Fig. 6.

Middle Section: Middle section consists of 3 perforated plates of 160 mm diameter, which are fitted as packing material at a distance of 0.5 m, 1.5 m and 1.7 m from the top of the scrubber as shown in Fig. 7.

Bottom Section: The bottom section consists of a 5 mm thick mild steel plate provided with 15 mm gas feeding pipe attached with a regulatory valve and a pressure gauge. The bottom plate is also provided with a 30 mm waste water outlet pipe fitted with a valve to control the flow as shown in Fig. 8. The top plate is bolted with the bottom plate by means of three tie rods of diameter 10 mm. Schematic diagram of top view with dimensions is shown in Fig.9.

Water supply system

A reciprocating pump is selected to supply water under pressure to the scrubber at low discharge. A 15 mm diameter GI pipe is fitted with a regulating valve to control the flow of water. To measure the pressure of water a pressure gauge is fitted as shown in Fig.10.

Gas supply system

Biogas is collected from the plant by means of a flexible balloon and stored in the vessel of a 1 kW two stage compressor with the suction capacity of 15 m^3/h. The biogas can be compressed up to 10 bar pressure before supplying to the scrubber as shown in Fig. 11. Pressure of gas in the vessel and supplied to the scrubber is measured by pressure gauges. A flexible pipe of 15 mm diameter is used to supply compressed biogas to the scrubber and the gas flow rate is controlled by a regulatory valve.

COST ESTIMATION OF WATER SCRUBBER

The following items are purchased for water scrubber from local market with reasonable price and the fabrication cost, transportation cost and labour cost are stated below in table 4.

STORAGE AND CLEANING OF ENRICHED BIOGAS

The purified biogas is collected from the outlet valve provided at the bottom of the scrubber by a flexible balloon for cooking and I.C. engine applications as shown in Fig. 12.

Cleaning of Biogas

Biogas contains traces of H_2S and moisture after the scrubbing, which cause corrosion of engine parts and cooking stoves [10, 3]. Hence proper elimination of these components to an acceptable level is to be carried out before supplying it to the I.C. engine and cooking application. The cleaning is done through the process of desulphurization to remove H_2S and dehydration to remove moisture.

Desulphurization

Hydrogen sulphide is a colorless, corrosive, poisonous and flammable gas with foul odor of rotten eggs [13]. Hydrogen sulphide is to be removed from biogas as it causes corrosion in the cooking stove and engine parts. Different methods are adopted to remove H_2S from biogas. In water scrubbing process some amount of H_2S is also removed along with CO_2. The most commonly used processes are dry oxidation process, liquid phase oxidation processes, membrane separation and biological treatment. The dry oxidation process used for H_2S removal is given below:

Dry oxidation using iron oxide

The biogas is passed through a desulphurizer as shown in Fig. 13, containing iron oxide as desulfurizing agent. The biogas desulphurizer consists of a container of dimensions 350 x 150 x 150 mm, 15 mm diameter soft pipe at inlet and outlet openings, a pressure gauge to measure between 0-10 bar and 2 kg of iron oxide as desulfurizing agent. The purified biogas is passed though the desulphurizer by the inlet pipe. Hydrogen sulphide is removed through chemical reaction as it reacts with iron oxide (Fe_2O_3) to form iron sulphide (Fe_2S_3) as shown in Eq. (1) [5].

$$Fe_2O_3 - 3H_2S = Fe_2S_3 + 3H_2O \quad (1)$$

The iron oxide is regenerated with oxygen according to the reaction in Eq. (2) by exposing it to the atmosphere to react with the atmospheric oxygen.

$$2Fe_2S_3 + 3O_2 = 2Fe_2O_3 + 6S \quad (2)$$

Dehydration

The presence of moisture in biogas causes corrosion and also reduces the heating value of the flame. Therefore, water vapor is to be removed before use. The most common method is dehydration process. In this process the purified biogas after desulphurization is passed through the dehydrator containing silica gel as shown in Fig. 14 to eliminate

the moisture present in it. The dehydrator introduces inlet and outlet points in the gas flow system, where moisture is absorbed by the silica gel from the biogas.

POWER COST FOR UPGRADING 1 m^3 OF BIOGAS

To store raw biogas in the compressor:	0.3 kWh
To run the reciprocating pump:	0.2kWh
Total power consumption:	0.5kWh
Power cost for1kWh:	USD 0.036
Total power cost for 1m^3	
Biogas enrichment:	USD 0.036

RESULTS AND DISCUSSIONS

A vertical floating drum type digester of 2 m^3 capacity has been installed to produce biogas from kitchen wastes. Raw biogas is collected by a flexible balloon of 1 m^3 capacity for purification purpose twice daily. A water scrubber has been designed and fabricated for removal of CO_2 from the raw biogas. It is found that the highest CO_2 removal is 88% at the gas flow rate of 1.5 m^3/h at 3 bar inlet pressure and water flow rate of 2 m^3/h at 4 bar pressure. The estimated cost of the water scrubber is Rs. 9,500/ only. The power cost of 1 m^3 biogas enrichment is Rs. 2.25/ only. The enriched biogas is used as fuel for cooking applications and as an alternate fuel in I.C. engines. A chromatography test has been carried out by using a Biogas Check Analyzer to find the different constituents of biogas before and after scrubbing as shown in Fig. 15. The results found by gas analyzer are shown in Figs. 16 and 17. The results of the biogas contents are provided in Table 5. Before scrubbing, the contents of CH_4, CO_2 and H_2S are found as 69.7%, 30.1% and 1236 ppm respectively. After scrubbing, the contents are found to be 96.3% for CH_4, 3.6% for CO_2 and 967 ppm for H_2S.

CONCLUSION

The study revealed that the designed and fabricated water scrubber is able to remove 89.74% of CO_2 present in raw biogas. The fabrication and maintenance cost of the scrubber is low. The power cost for enrichment of biogas is low. The enriched biogas containing 96.3% of CH4 is used as fuel for cooking and as an alternate fuel in I.C. engines. This enrichment unit can be installed in the areas where large quantities of organic wastes and sufficient water are available.

REFERENCES

1. Augelletti, R., Conti, M., Annesini, M.C., 2017, "Pressure swing adsorption for biogas upgrading; A new process configuration for the separation of biomethane and carbon dioxide", *J. Clean. Prod.* 140,1390–1398.
2. Ashare, E. and Wilson, E., 1978, "Evaluation of systems for purification of fuel gas from anaerobic digestion", *Dynatech. R/D Company Rep. 1628, U.S. Department ofEnergy.*
3. Agrawal, K. M., B. R. Barve, Khan, S. S., 2010, "Biogas from press mud," *IOSR Journal of Mechanical and Civil Engineering (IOSR- JMCE),* 4(45), pp.37-41.
4. Block, D. et al., 1986, "Recovery of Methane from Biogases", *Energy from Biomass Biogas generation etc.* 1stE.C.Conf.
5. Gaikwad, V.R. and Katti, P. K., 2014, "Design of biogas scrubbing, compression & storage system", *IOSR Journal*

of Electrical and Electronics Engineering, 1(2), pp.58-63.

6. Jensen-Holm, C., 1983, "Biogas Purification".
7. Kohl, A.L. and Nielsen, R. B., 1985, "Gas Purification", 4th*ed., Gulf Publishing, Houston,Texas.*
8. Kennes, D., Abubackar, H.N., Diaz, M., Veiga, M.C., Kennes, C., 2016, "Bioethanol production from biomass: carbohydrate vs syngas fermentation" *J. Chem. Technol. Biotechnol.* 91, 304–317.
9. Kougias, P.G., Campanaro, S., Treu, L., Zhu, X., Angelidaki, I., 2017, "A novel archaeal species belonging to methanoculleus genus identified via de-novo assembly and metagenomic binning process in biogas reactors", *Anaerobe,* 46,23–32.
10. Lien, C.C., Lin, J. L., Ting, C. H., 2014, "Water scrubbing for removal of hydrogen sulphide in biogas from hog farms," *Journal of Agricultural Chemistry and Environment,* 3(1), pp.1-6.
11. Mohanty, M.K., 2012, "Biogas application in rural industries", *LAP Lambert academic publishing.*
12. Schomaker,Ir.A.H.H.M.,Boerboom,ing.A.M., Visser, ir. A., Pfeifer, ing. A. E., 2000, "Technical summary on gas treatment, Anaerobic digestion of agro-industrial wastes", *Information networks, Project FAIR*-CT96- 2083(DG12-SSMI).
13. Strickland, J., Cummings, A., Spinnato, J. A., 2003, "Toxicological review of hydrogen sulphide", *Tech. Rep. 7783, U.S. Environmental Protection Agency,* Washington, DC.
14. Sun, Q., Li, H., Yan, J., Liu, L., Yu, Z., Yu, X., 2015, "Selection of appropriate biogas upgrading technology-a review of biogas cleaning, upgrading and utilization", *Renew. Sust. Energy Rev.* 51,521–532.

Table 1. Biogas Utilization and Purification [6]

Biogas Utilization	H_2S Removal	CO_2 Removal
Cooking	Yes	No
Domestic heating	No	No
Boilers	Depends	No
Vehicles	Yes	Yes
Delivery to natural gas	Yes	Yes
Transportation	Yes	Yes

Table 2. Scrubber design

Designparameters	Specification
Plant capacity	2 m^3
Plantefficiency	50%
Biogas produced	1 m^3/day
% of methane in raw biogas	69%
% of methane in scrubbed gas	96%
Diameter of scrubber	150 mm
Height of scrubber	3000 mm
Number of stages	3
Pressure of biogas	3 bar
Pressure of water used forscrubbing	4 bar

Table 3 Parameters and specifications of scrubbing tower

Designparameters	Specification	Designparameters	Specification
Height of the scrubbing tower	3000 mm	Thickness of transparent fibre cylinders	5 mm
Diameter of the scrubbing tower	150 mm	Number of transparent fibre cylinders	3
Supporting frame with stand fabricated by square bar.	40 mm	Diameter of tie rods	10 mm
Diameter of transparent fibre cylinders	150 mm	Number of tierods	3
Length of each transparent fibre cylinders	1000 mm		

Table 4 Cost estimation of water scrubber

Sl. No.	Description	Cost in USD
1	Raw materials of supporting frame and fabrication	14.29
2	Transparent fibre cylinders (3 nos.)	21.44
3	Mild steel tie rods with nuts and bolts for top and bottomplates	4.28
4	Top and bottom section mild steel plates	2.85
5	Water spraying nozzle	4.28
6	Packing materials	2.85
7	Pressure gauge (2 nos.) and a regulatory valve (3nos.)	21.44
8	GI pipe of 15 mm & 30 mm diameter with fittings	35.73
9	Transportation cost and labour cost	28.58
	Total estimated cost	135.74

Table 5 Biogas analysis results obtained by chromatography

Sample Location	CH4 (%)	CO2 (%)	H2S (ppm)
Raw Biogas	69.7	30.1	1236
Purified Biogas	96.3	3.6	967

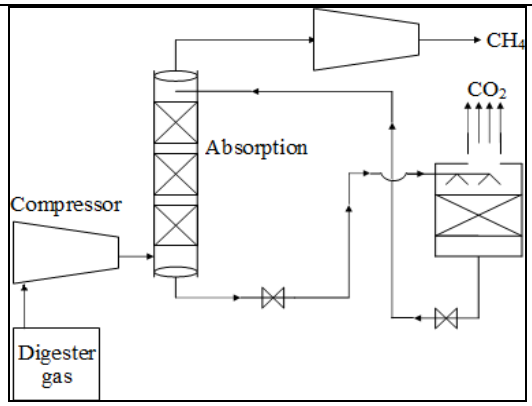

Fig. 1 Flow diagram of water absorption method [11]

Fig. 2 Water scrubber

Fig. 3 Biogas enrichment unit

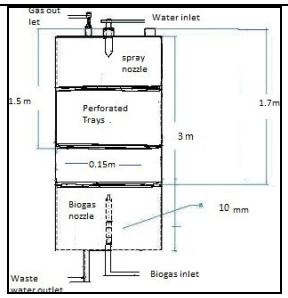

Fig. 4 Schematic view of the scrubbing tower

Fig. 5 Top section of the scrubber

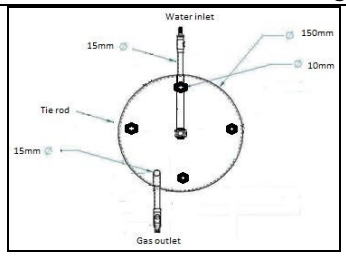

Fig. 6 Top view of scrubber

Fig. 7 Middle section of the scrubber

Fig. 8 Bottom section of the scrubber

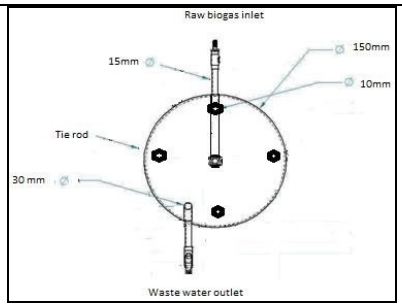

Fig. 9 Bottom view of scrubber

Fig. 10 Reciprocating pump

Fig. 11 Raw biogas compression and storage

Fig. 12 Storage of enriched biogas

Fig. 13 Biogas desulphurizer

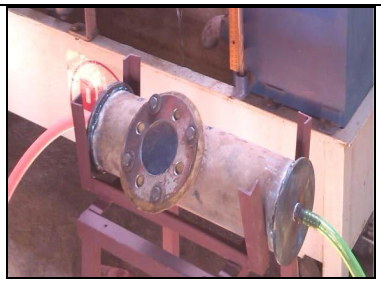

Fig.14 Biogas dehydrator

Fig. 15 Biogas check analyzer

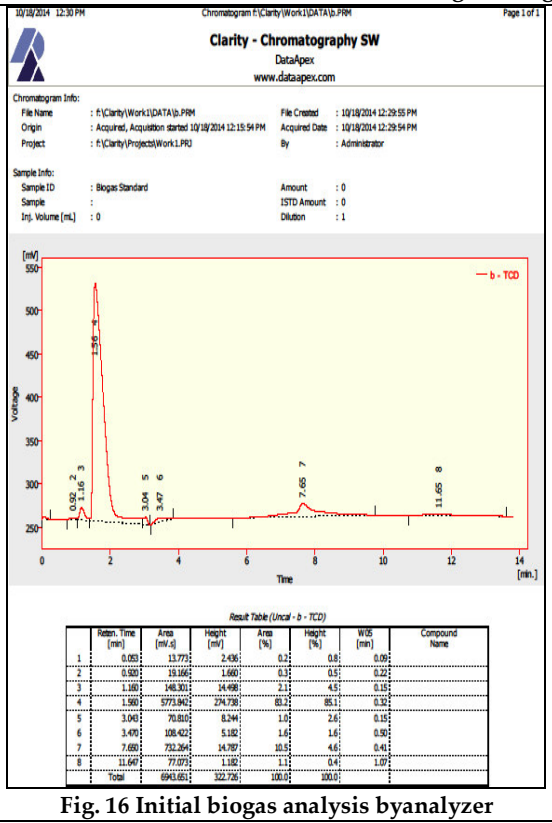

Fig. 16 Initial biogas analysis byanalyzer

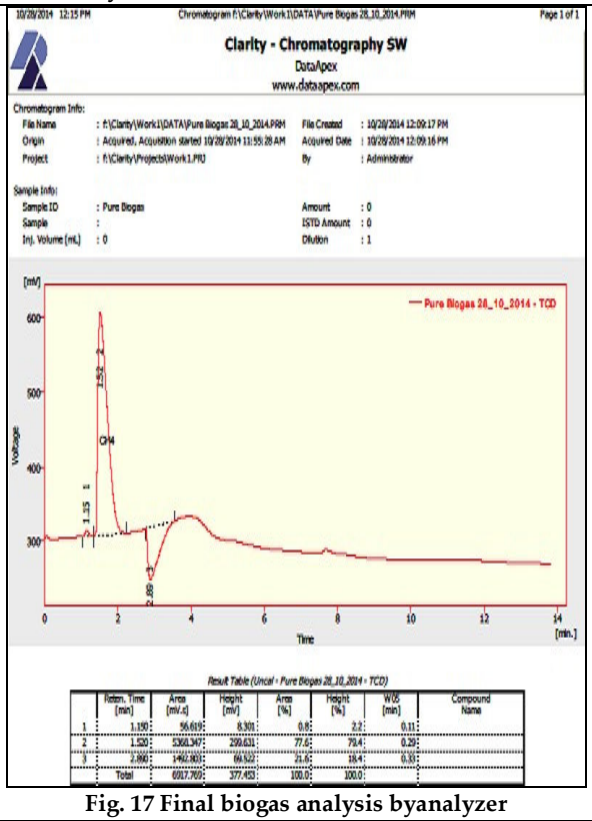

Fig. 17 Final biogas analysis byanalyzer

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RESEARCH ARTICLE

Ab-Initio Calculations of Electronic Properties of Terbium Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties likehighspeed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiCwas doped with Terbium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Terbium doping on SiC.

Keywords: manner, structure, Terbium, energies

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN(3.4eV), diamond (5.5eV),ZnS(3.6eV) etc.Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme

environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand, the wide bandgap semiconductors (e.g. SiC,GaN and ZnOetc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties. Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiCcrystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high-power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. Its properties have made SiC a research focus till date [3,4,5]. This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC.Then, SiC was doped with Terbium and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., BIOVIA. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials[6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work.BIOVIA Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger[8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels.The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Terbium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Terbium atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undopedSiC and doped SiC with Terbium are compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubiccrystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is shown inFig. 2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in

the form 2x2x1in X-, Y- and Z-direction. The corner Silicon atom is replaced with Terbium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Terbium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort.
The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6. shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undopedSiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 8. showed the many peaks but the maximum peak is at 8.2 eV. Fig. 9 shows the band energy plot for SiC doped with Terbium in the supercell calculation. Here top of valence band is taken as zero. From the fig it is observed that top of valence band and bottom of conduction band occurs at one point showing direct band gap. This indicates a change in the behavior of Terbium doped SiC than pure SiC. Fig. 10 shows the DOS plot for SiC doped with Terbium in the supercell calculation. From the fig it is observed that SiC after doping with Terbium its band gap decreases, and almost it looks like a continuous plot which probably indicate metallic behavior. A sharp peak is observed exactly on the Fermi energy level. This indicates the presence of charge carriers at Fermi level.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC.All these were also done for SiC doped with Terbium. The calculations were done using the Dassault system BIOVIA-Material Studio.Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Terbium doped SiC.From the DOS plot it is observed that SiC after doping with Terbium its band gap decreases, and almost it looks like a continuous plot which indicate metallic behavior. A sharp peak is observed exactly on the Fermi energy level. This indicates the presence of charge carriers at Fermi level.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
A. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
2. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, ChunmingNiu and ShouwuGuo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
3. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
4. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
5. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
6. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
7. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-
8. electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn,Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

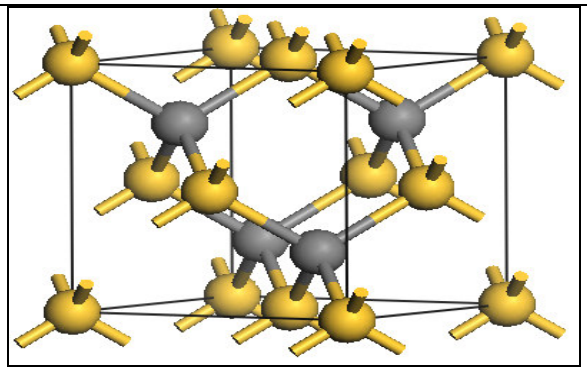

Figure 1: Crystal structure ofSiC

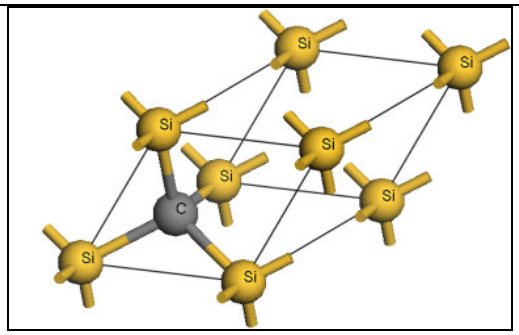

Figure 2: Primitive cell of SiC

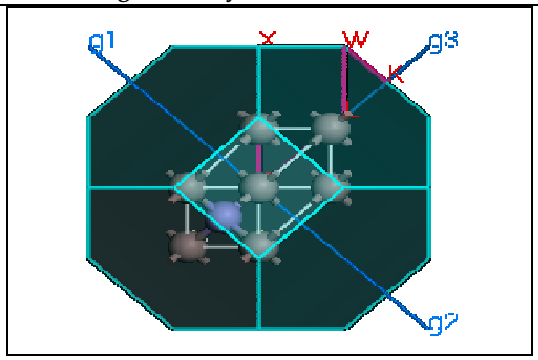

Figure 3:Brillouine zone of SiCFigure

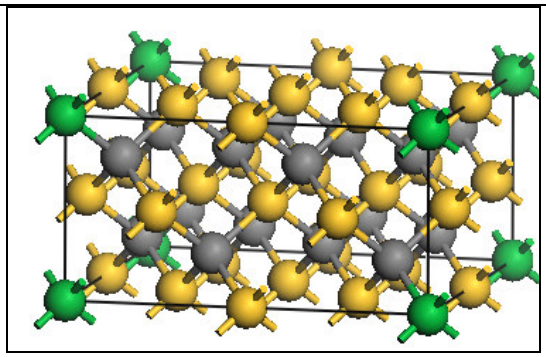

Figure 4:Terbium doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and green color for Terbium atoms.

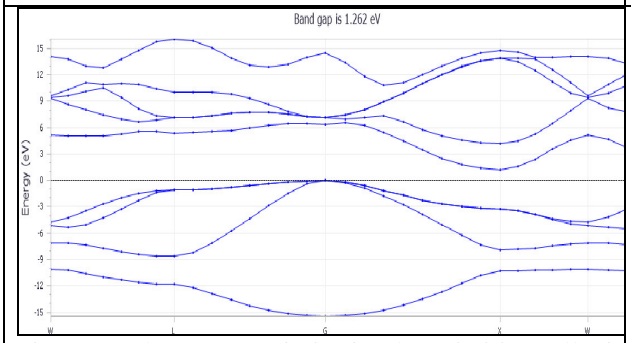

Fig 5. :Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

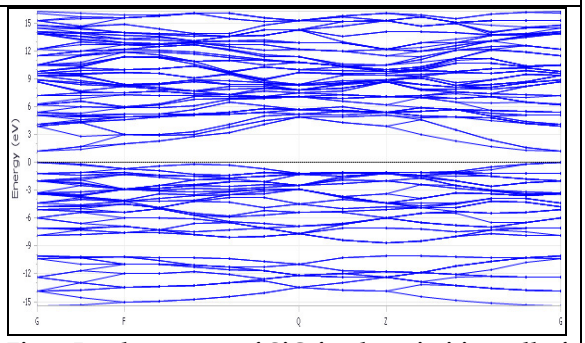

Fig 6. Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

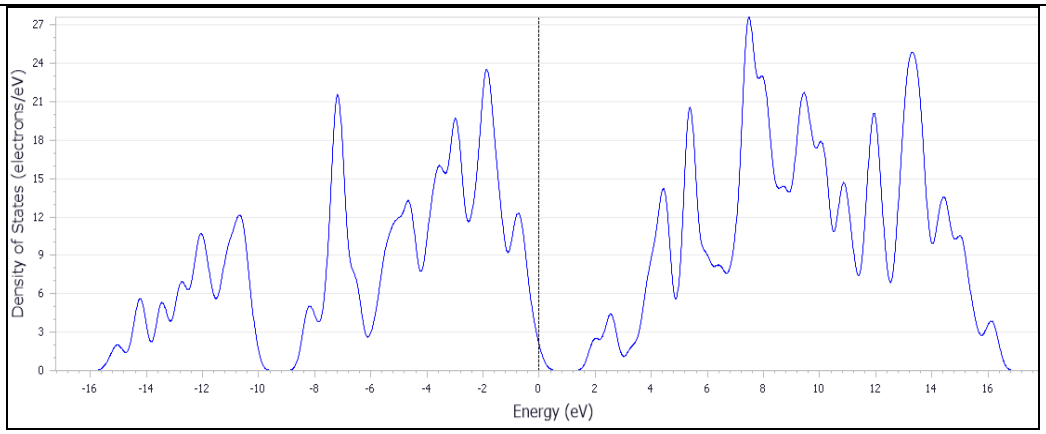

Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

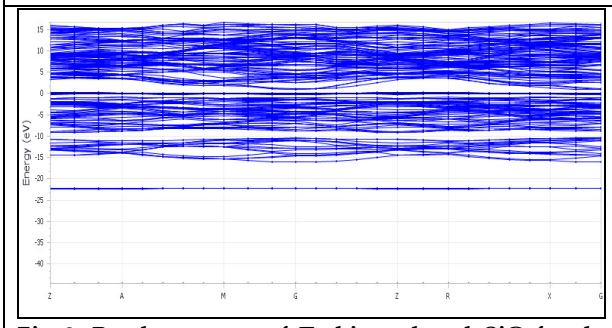

Fig 8: Band structure of Terbium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

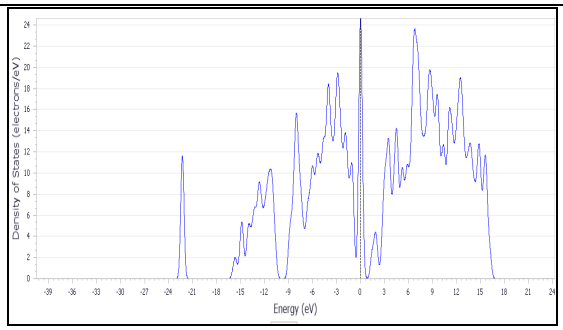

Fig 9 :Density of states of Terbium doped SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Ab Initio Study of Electronic Properties of Samarium Doped Silicon Carbide

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ABSTRACT

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Keywords: Density, Samarium, electronics, properties, SiC

INTRODUCTION

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replaced with Samarium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Samarium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort.

The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap. The total density of states (DOS) of undoped SiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 8 showed the many peaks but the maximum peak is at 8.2 eV.

Fig. 9 shows the band energy plot for SiC doped with Samarium in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that the band gap vanishes after doping with Samarium. This indicates a change in the behavior ofSm doped SiC than pure SiC.Fig. 9 shows the DOS plot for SiC doped with Samarium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the band gap is zero after doping withSamarium. A sharp peak is seen on the Fermi energy level. The distribution of electrons in the valence and conduction band is found to be same in both undoped and doped cases. The band gap between valence and conduction band becomes 0. The DOS plot show many peaks but it has a maximum peak at 6.60ev. After doping with Samarium,SiC shows metallic behavior.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for

SiC. All these were also done for SiC doped with Samarium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Sm doped SiC. The band gap decreases to zero after doping witSamarium and it shows metallic behavior. This indicates a change in the behavior of Sm dopedSiC than pure SiC. This is an interesting result and it will be further interesting to verify the properties by increasing the percentage of doping.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
A. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
2. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
3. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
4. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
5. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
6. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
7. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
8. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
9. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
10. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
11. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
12. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
13. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
14. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

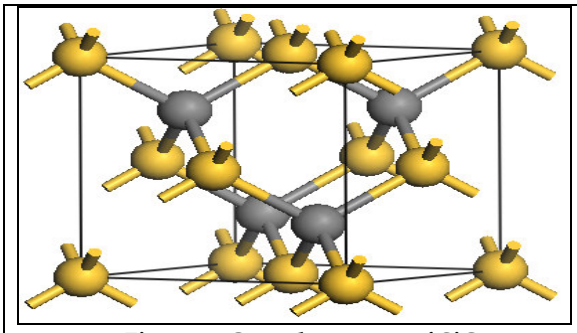


Figure 1: Crystal structure of SiC

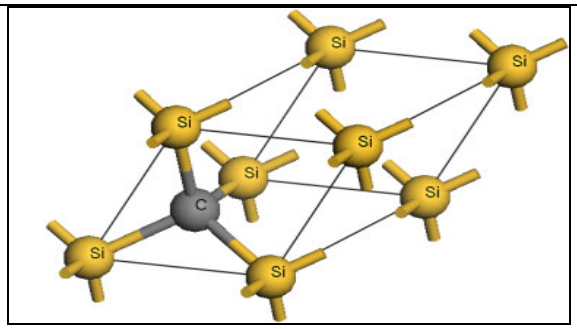


Figure 2: Primitive cell of SiC Si in yellow and C in grey.

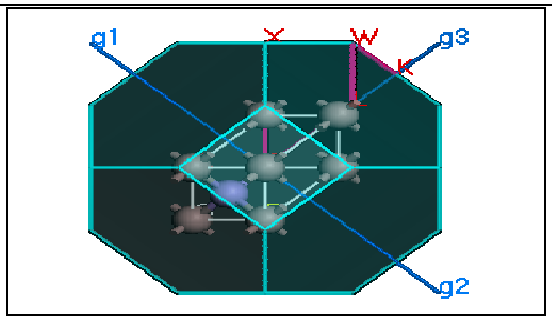


Figure 3: Brillouine zone of SiC

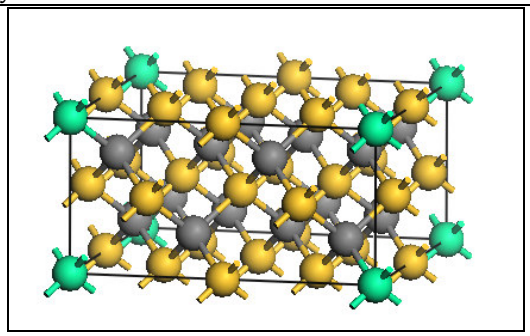


Figure 4:Samarium doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Green is for Samarium atoms.

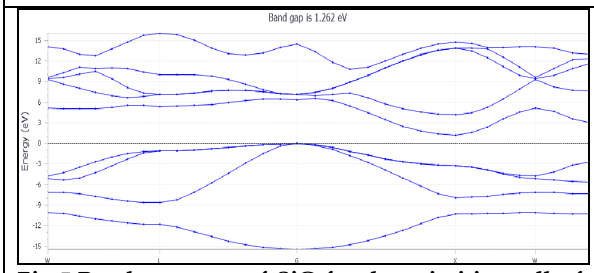


Fig 5.Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

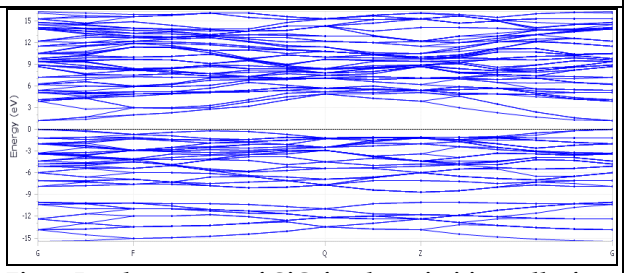


Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

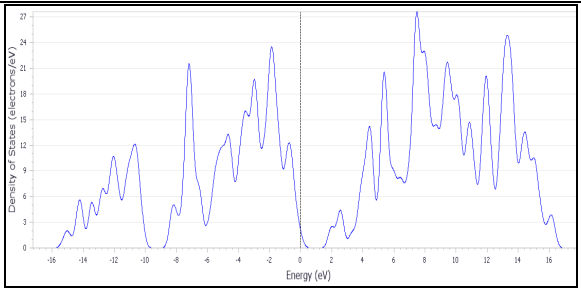


Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

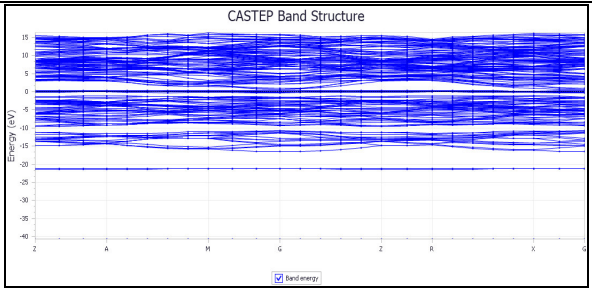
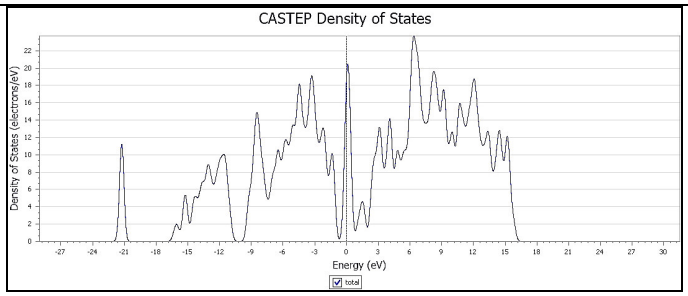


Fig 8. Band structure of Samarium dopedSiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.



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RESEARCH ARTICLE

Ab-initio Study of Electronic Properties of Silver Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties likehighspeed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiCwas doped with Silver and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Silver doping on SiC.

Keywords: semiconductor, power, materials, Silver

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN(3.4eV), diamond (5.5eV),ZnS(3.6eV) etc.Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme

environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand, the wide bandgap semiconductors (e.g. SiC,GaN and ZnOetc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties. Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiCcrystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high-power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2].Its properties have made SiC a research focus till date [3,4,5]. This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC.Then, SiC was doped with Silver and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., BIOVIA. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials[6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work.BIOVIA Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

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Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

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Fig. 8 shows the band energy plot for SiC doped with Silver in the supercell calculation. Here top of valence band is taken as zero. By analyzing the graph, it is found that, SiC after doping with Silver its band gap decreases almost equal to zero. This negligible band gap indicates change in conductivity. Comparing this with the energy bands shown in Fig. 6, it is observed that the band gap changes after doping with Silver. Fig. 9 shows the DOS plot for SiC doped with Silver in the supercell calculation. From the plot it is observed that there is no gap between the conduction band and valence band that means the curve is continuous which may indicate towards metallic behavior. The Fermi level has shifted up and located between the conduction band and valence band. Small peaks are seen on and near the Fermi level.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiC was done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for

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REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
A. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
2. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, ChunmingNiu and ShouwuGuo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
3. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
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5. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
6. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
7. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
8. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
9. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
10. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
11. P. Hohenberg and W. Kohn,Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
12. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
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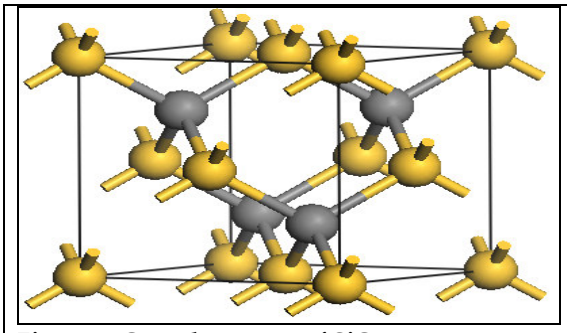

Figure 1: Crystal structure of SiC

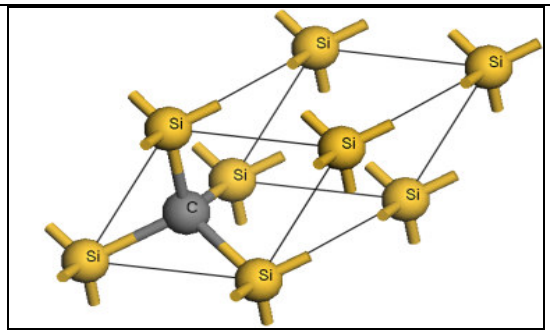

Figure 2: Primitive cell of SiC Si in yellow and C in grey.

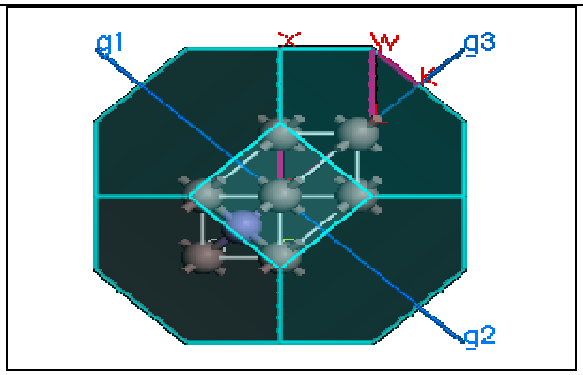

Figure 3: Brillouine zone of SiC

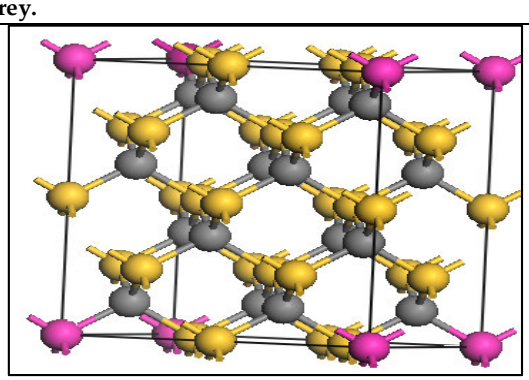

Figure 4:Silver doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Pink is for Silver atoms.

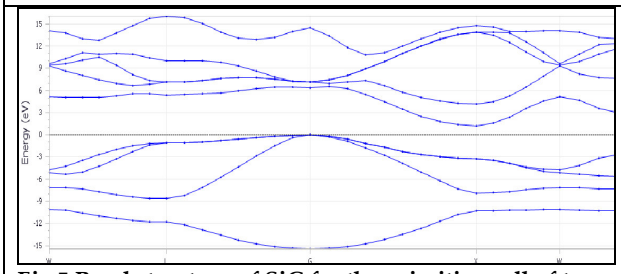

Fig 5.Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

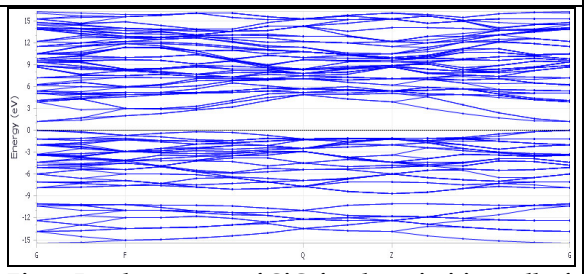

Fig 6. Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

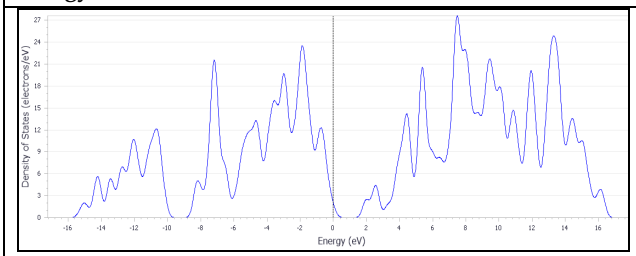

Fig 7.:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

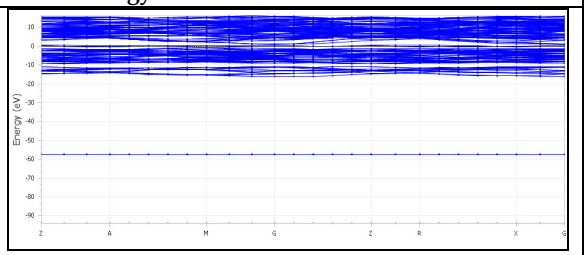

Fig 8. Band structure of Silver doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

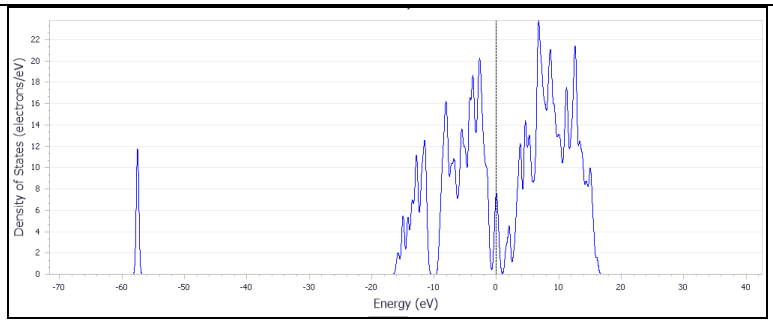

Fig 9 Density of states of Silver doped SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Ab-Initio Study of Electronic Properties of Technetium Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties likehighspeed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Technetium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Technetium doping on SiC.

Keywords: electrical, Technetium, parameters, temperature

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN(3.4)eV), diamond (5.5eV),ZnS(3.6eV) etc.Silicon has

ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC,GaN and ZnOetc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5].

This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC. Then, SiC was doped with Techentium and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials[6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger [8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels.The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Techentium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undoped SiC and doped SiC withTechentiumare compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubiccrystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is shown inFig. 2 and the BZ sampling is shown in Fig..3. A supercell was created by expanding the lattice constant in the form 2x2x1in X-, Y- and Z-direction. The corner Silicon atom is replaced with Techentium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Techentium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort.

The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap. The total density of states (DOS) of undoped SiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV.

Fig. 8 shows the band energy plot for SiC doped with Techentium in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that the band gap decreases after doping with Techentium.Fig. 9 shows the DOS plot for SiC doped with Techentium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the decrease in band gap is associated with a shifting of the Fermi energy level. The Fermi energy level is located inside the conduction band. The distribution of electrons in the valence band has changed in the presence of the impurity.The DOS plot show many peaks but it has a maximum peak at 6.20ev.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Technetium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows. The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Tc doped SiC. The band gap decreases to zero after doping with Technetium and it shows metallic behavior. This indicates a change in the behavior of Tc doped SiC than pure SiC. This is an interesting result and it will be further interesting to verify the properties by increasing the percentage of doping.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
A. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
2. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
3. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
4. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
5. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
6. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
7. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
8. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
9. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
10. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
11. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
12. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
13. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
14. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

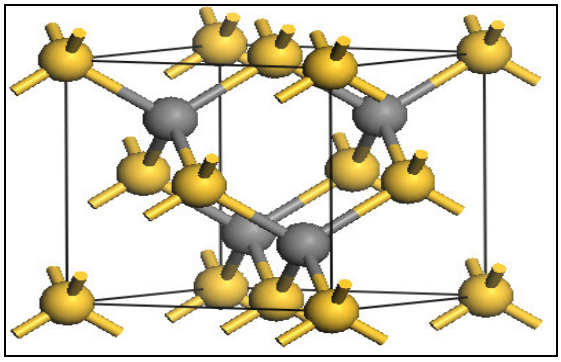


Figure 1: Crystal structure of SiC

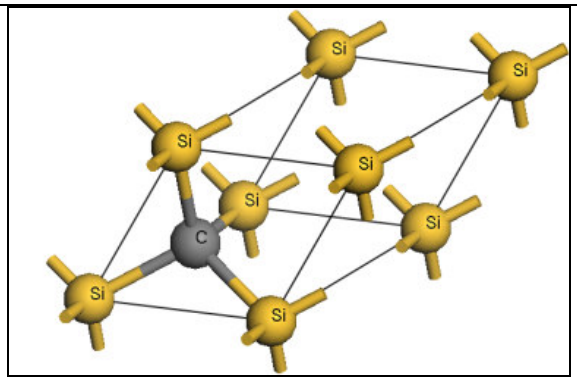


Figure 2: Primitive cell of SiC Si in yellow and C in grey.

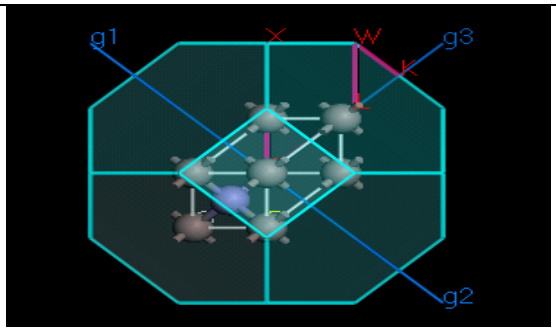


Figure 3: Brillouine zone of SiC

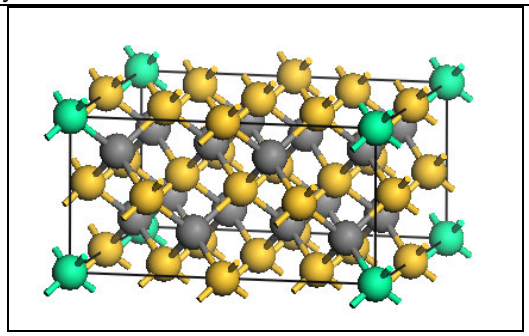


Figure 4:Technetiumdoped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Green is for Technetium atoms.

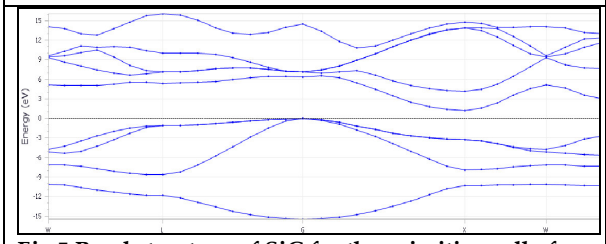
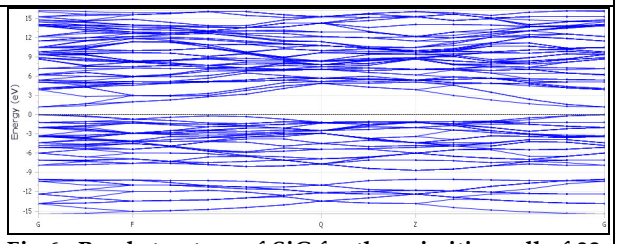


Fig 5.Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.



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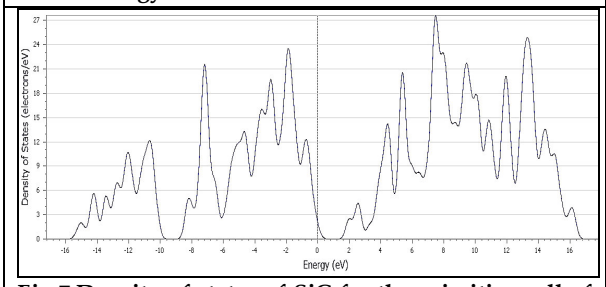


Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

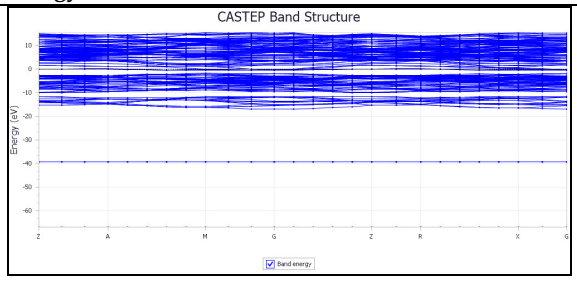
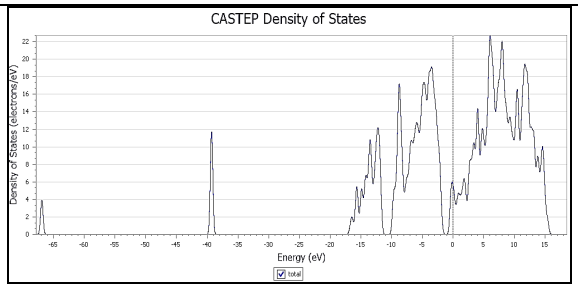


Fig 8: Band structure of Technetium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.



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RESEARCH ARTICLE

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We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell. More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undopedSiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 8 shows the band energy plot for SiC doped with Titanium in the supercell calculation. Comparing with the energy bands shown in Fig. 6 it is observed that the band gap decreased after doping with Titanium. The distribution of electrons in the valence and conduction band is more towards the both sides of bandgap. This indicates a possible change in the behavior of Ti doped SiC than pure SiC.Fig. 9 shows the DOS plot for SiC doped with Titanium in the supercell calculation. Comparing with the DOS plot shown in Fig. 3.3, it is observed that the band gap decreased slightly after doping with Titanium. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence and conduction band is different in undoped and doped cases.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Titanium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observationscan be summarized as follows. The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Ti doped SiC. The band gap remains the same before and after doping with Titanium. But the indirect band gap of SiC has now changed to direct band gap. This indicates a change in the behavior of Ti doped SiC than pure SiC. We observed that the band gap decreased after doping with Titanium. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence and conduction band is more towards the both sides of bandgap.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).

15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL **1999**

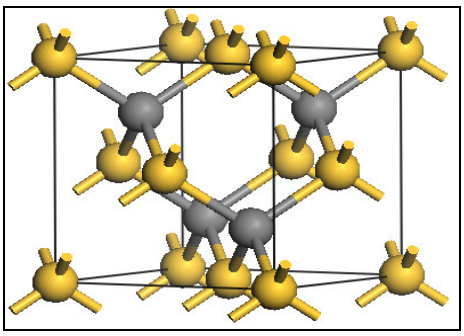

Figure 1: Crystal structure of SiC

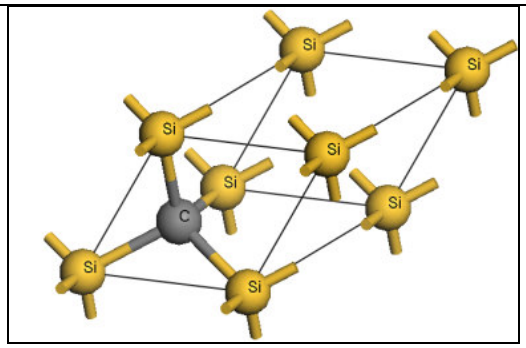

Figure 2. Primitive cell of SiC Si in yellow and C in grey.

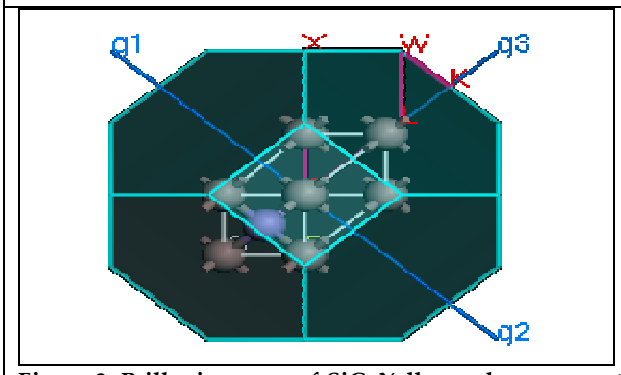

Figure 3: Brillouine zone of SiC .Yellow color represents Si atom, Grey is for C atoms and Pink is for Titanium atoms.

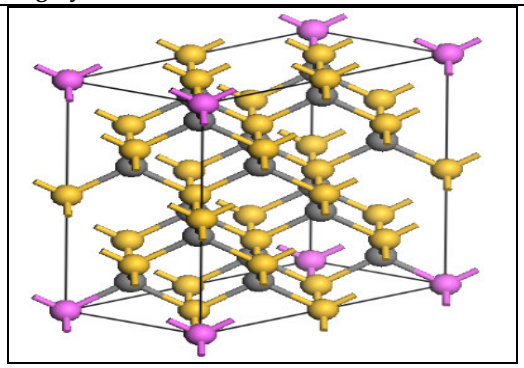

Figure 4:Titanium doped SiC supercell.

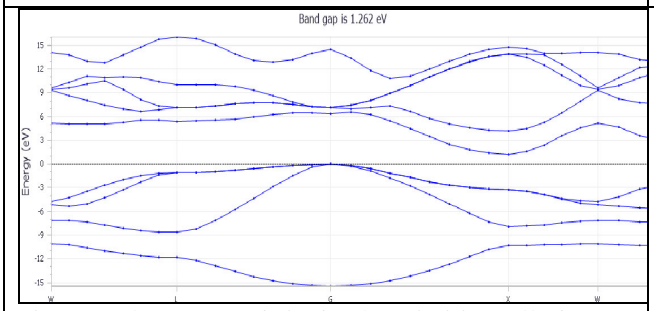

Fig 5:Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

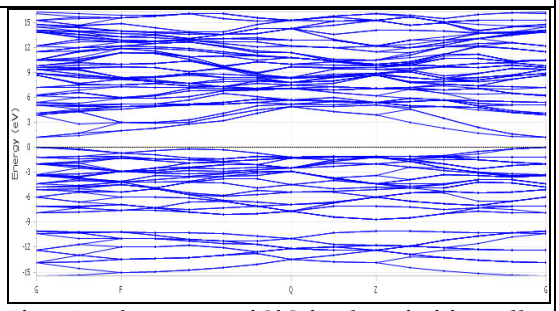

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

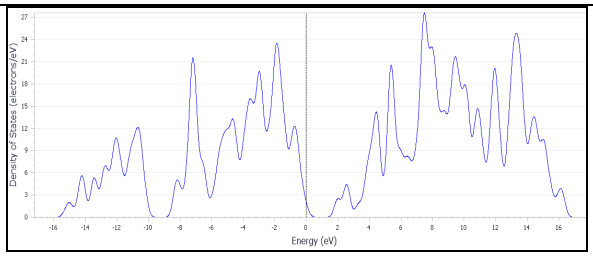

Fig 7: Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

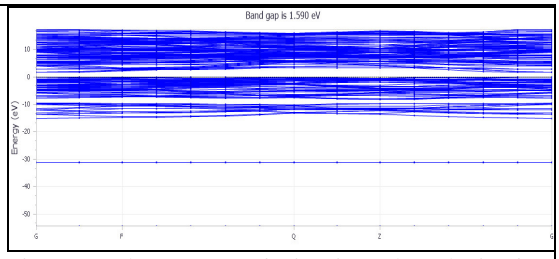

Fig 8: Band structure of Titanium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

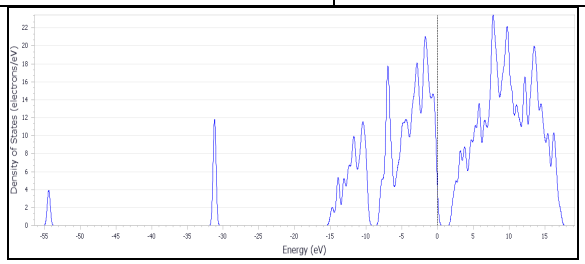

Fig 9.Density of states of Titanium dopedSiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Computational Study of Indium Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like high speed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Indium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Indium doping on SiC.

Keywords: electrical, Indium, doping, Density, semiconductor

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC (band gap:2.3 to 3.4 eV), GaN (3.4)eV), diamond (5.5eV), ZnS (3.6eV) etc. Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors,

shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC, GaN and ZnO etc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8 V/m for different polytypes), high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high power devices to operate in higher value of blocking voltage. High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5]. This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC. Then, SiC was doped with Indium and the changes after adding the impurity was observed by comparing the undoped and doped results. The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials [6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger [8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels. The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Indium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Indium atom is placed in place of Si atom. So the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undoped SiC and doped SiC with Indium are compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubic crystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is

shown in Fig. 2.2 and the BZ sampling is shown in Fig. 2.3. A supercell was created by expanding the lattice constant in the form 2x2x1 in X-, Y- and Z-direction. The corner Silicon atom is replaced with Indium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Indium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiC were done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 3.1. The top of the valence band is taken as 'zero' along the energy axis. The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating an indirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA. Fig. 3.2 shows the band plot for SiC with 32 atoms in the primitive cell. More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undoped SiC using first principle DFT with LDA using pseudopotential are shown in Fig. 3.3. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 3.3 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 3.4 shows the band energy plot for SiC doped with Indium in the supercell calculation. Comparing with the energy bands shown in Fig. 3.2, it is observed that the band gap decreases slightly after SiC is doped with Indium . It implies that there is an appreciable shift of electric properties of In doped SiC than that of pure SiC. Fig. 3.5 shows the DOS plot for SiC doped with Indium in the supercell calculation. Comparing with the DOS plot shown in Fig. 3.3, it is observed that the band gap of SiC is decreased slightly after doping with Indium. There is no change in Fermi levels and its still located towards the top of the valence band.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiC was done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Indium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation. The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for In doped SiC. The band gap of SiC decreases after doping with Indium indicating the change in the electronic behaivour of Indium doped SiC than pure SiC. No change observed in the position of the Fermi level.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
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6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
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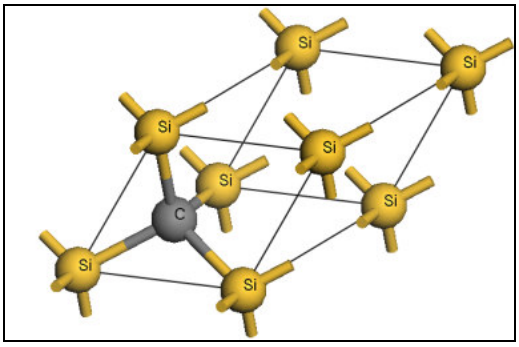

Figure 1: Crystal structure of SiC

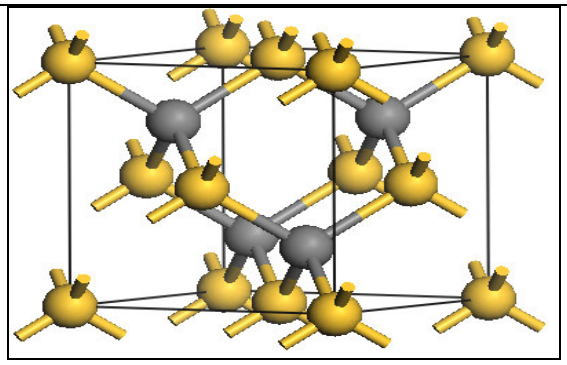

Figure 2: Primitive cell of SiC Si in yellow and C in grey.

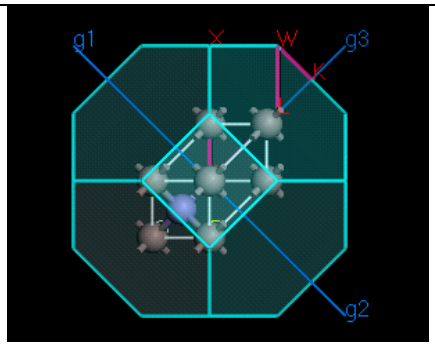

Figure 3: Brillouine zone of SiC

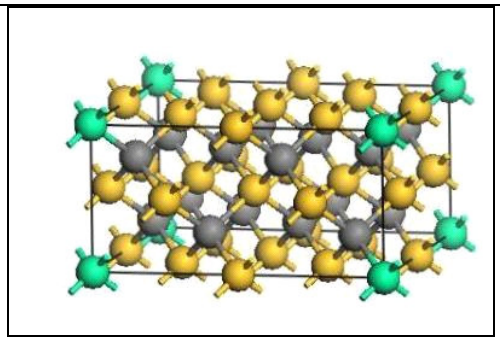

Figure 4: Indium doped SiC supercell. Yellow color Represents Si atom,Grey is for C and green is for In

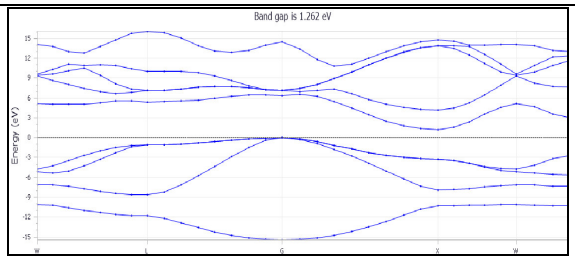

Fig 5:Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

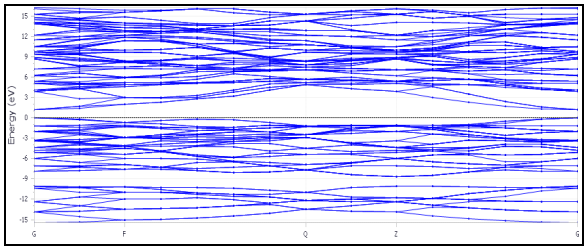

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

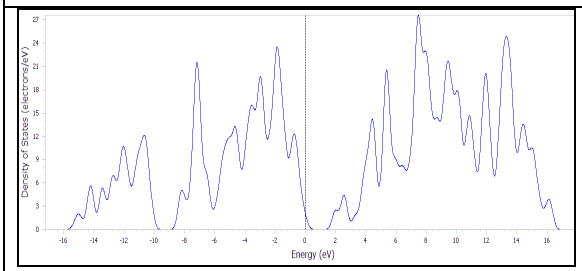

Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

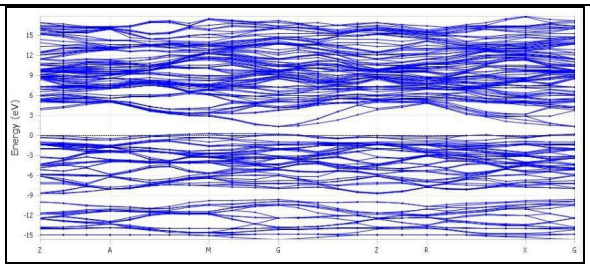

Fig 8: Band structure of Titanium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

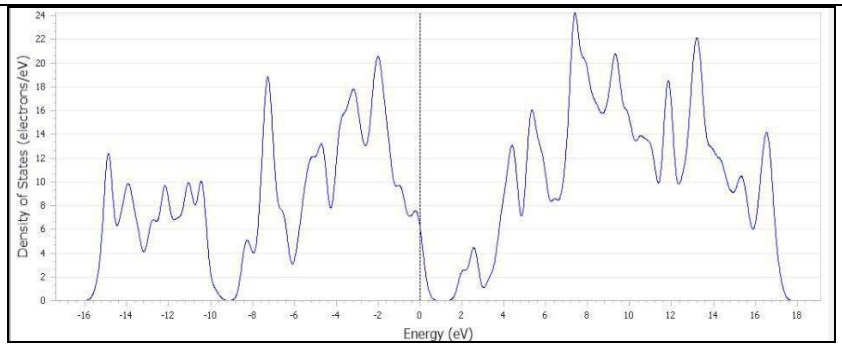

Fig 9: Density of states of Titanium dopedSiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Density Functional study of Dysprosium Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like highspeed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Dysprosium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Dysprosium doping on SiC.

Keywords: SiC, Theory, Dysprosium, electronics, highspeed, materials

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN(3.4)eV), diamond (5.5eV),ZnS(3.6eV) etc.Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors,

shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC,GaN and ZnOetc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiCcrystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC,can enable the high power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5].This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC.Then, SiC was doped with Dysprosium and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials[6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work.Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger[8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels.The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Dysprosium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Dysprosium atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undopedSiC and doped SiCwith Dysprosium are compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubiccrystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is

shown inFig.2 and the BZ sampling is shown in Fig.3. A supercell was created by expanding the lattice constant in the form 2x2x1in X-, Y- and Z-direction. The corner Silicon atom is replaced with Dysprosium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Dysprosium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undopedSiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 8 shows the band energy plot for SiC doped with Dysprosium in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that after doping with Dysprosium, the conduction band and valence band overlap each other, thus giving zero band gap. This may create a change in the behavior of Dy doped SiC than pure SiC.Fig. 9 shows the DOS plot for SiC doped with Dysprosium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the energy states are continuous with several peaks in place of the previous band gap. That means the band gap vanishes after doping with Dysprosium.The distribution of electrons in the valence has changed. The lower portion is almost empty while the upper portion of the valence band is occupied with the charge carriers.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC.All these were also done for SiC doped with Dysprosium. The calculations were done using the Dassault system BIOVIA-Material Studio.Our observations can be summarized as follows.The lattice constant of SiC is calculated

with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Dy doped SiC. The band gap vanishes after doping with Dysprosium as the conduction band and valence band ovelapwoth each other. This may lead to a change in the conducting properties of Dy doped SiC than pure SiC. This is an interesting result and it will be further interesting to verify the properties by increasing the percentage of doping.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, ChunmingNiu and ShouwuGuo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn,Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

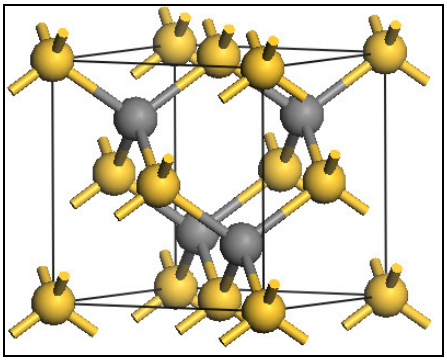

Figure 1: Crystal structure of SiC

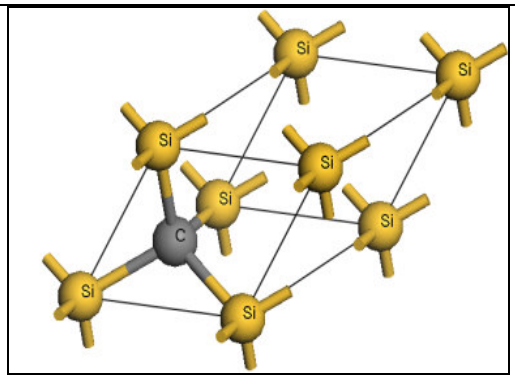

Figure 2: Primitive cell of SiC Si in yellow and C in grey.

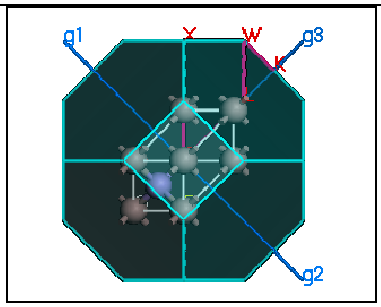

Figure .3: Brillouine zone of SiC Yellow color represents Si atom, Grey is for C atoms and Green is for Dysprosium atoms.

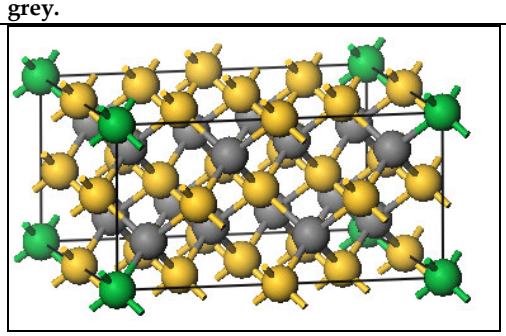

Figure 4:Titanium doped SiC supercell.

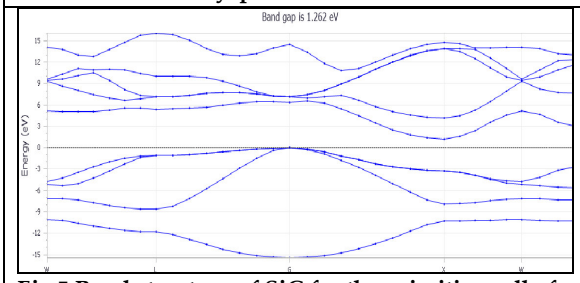

Fig 5:Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

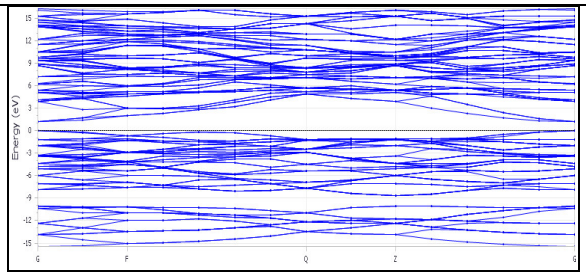

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

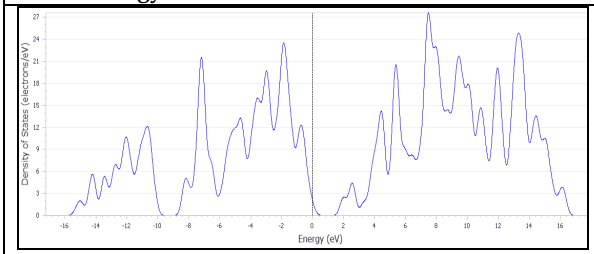

Fig 7: Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

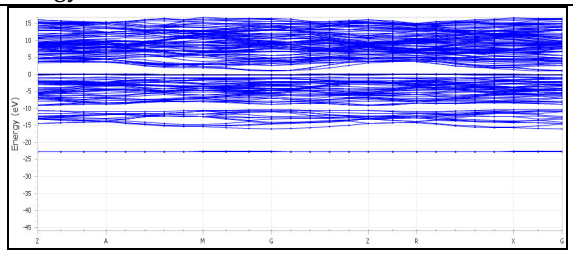

Fig 8 Band structure of Dysprosium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

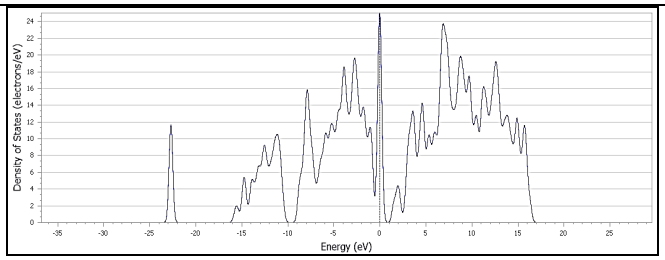

Fig 9. Density of states of Titanium dopedSiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Electronic Properties of Selenium Doped Silicon Carbide – A Computational Approach

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ABSTRACT

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Keywords: work, Selenium, structure, temperature, bandgap, SiC

INTRODUCTION

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CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiCdoped with Selenium.The calculations were done using the Dassault system BIOVIA-Material Studio.Our observations can be summarized as follows. The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Se doped SiC. The band gap has not changed much after doping with Selenium. The Fermi energy level is located inside the conduction band after doping. This indicates the increase in the highest occupied energy level. The distribution of electrons in the valence and conduction band is also same in both undoped and doped cases. The DOS plot show many peaks but it has a maximum peak at 5.60ev.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

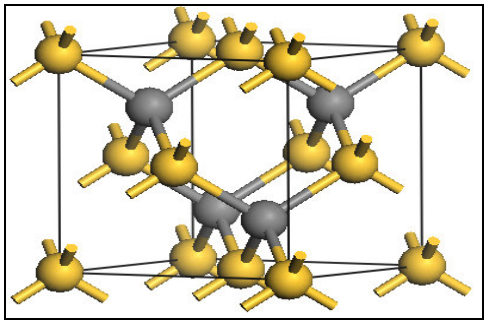

Figure 1: Crystal structure of SiC

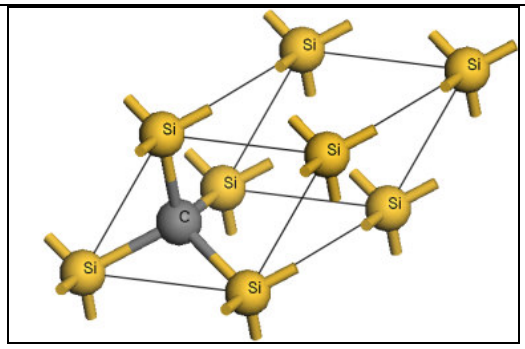

Figure 2: Primitive cell of SiC Si in yellow and C in grey.

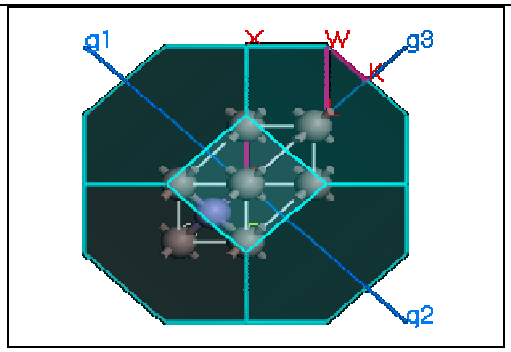

Figure .3:Brillouine zone of SiC

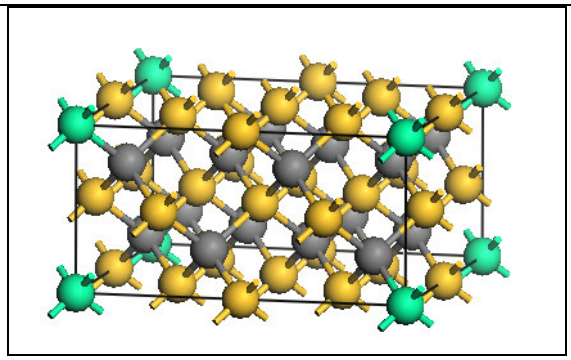

Figure 4: Seleniumdoped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Green is for Selenium atoms.

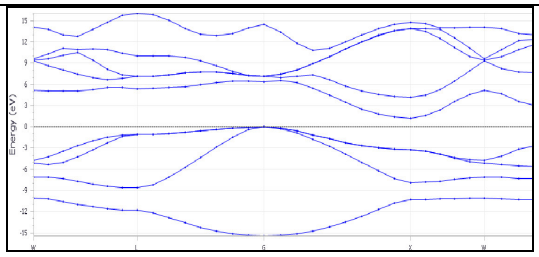

Fig 5.Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

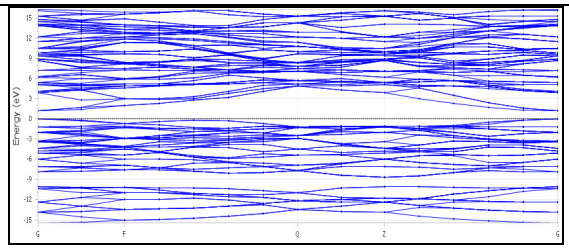

Fig 6.: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

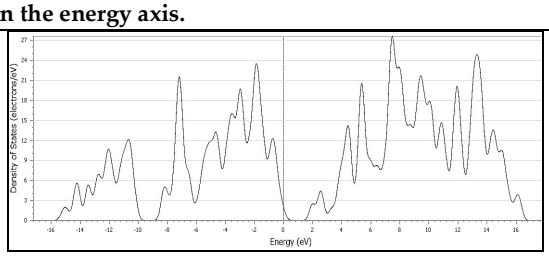

Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

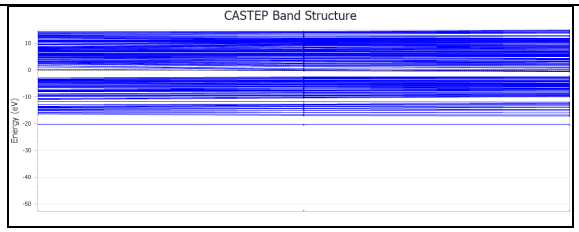

Fig 8: Band structure of Selenium dopedSiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

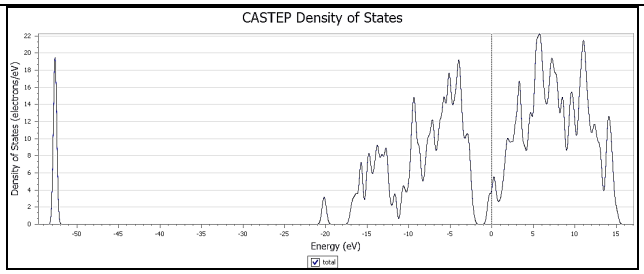

Fig 9 Density of states of Titanium dopedSiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Electronic Properties of Thorium Doped Silicon Carbide – A Computational Approach

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like high speed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Thorium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Thorium doping on SiC.

Keywords: parameters, Thorium, microprocessors, electronics, diamond

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC (band gap:2.3 to 3.4 eV), GaN (3.4)eV), diamond (5.5eV), ZnS (3.6eV) etc. Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors,

shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC, GaN and ZnO etc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8 V/m for different polytypes), high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high power devices to operate in higher value of blocking voltage. High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5].This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC. Then, SiC was doped with Thorium and the changes after adding the impurity was observed by comparing the undoped and doped results. The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials [6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger [8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels. The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Thorium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Thorium atom is placed in place of Si atom. So the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undopedSiC and doped SiC with Thorium are compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubic crystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is

shown in Fig. 2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in the form 2x2x1 in X-, Y- and Z-direction. The corner Silicon atom is replaced with Thorium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Thorium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiC were done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis. The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating an indirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA. Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell. More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undopedSiC using first principle DFT with LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 8 shows the band energy plot for SiC doped with Thorium in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that there is nearly an overlap of the bands after SiC is doped with Thorium . It implies that there maybe an appreciable shift of electric properties of Th doped SiC than that of pure SiC. Fig. 9 shows the DOS plot for SiC doped with Thorium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the band gap of SiCvanishes after begin doped with Thorium. With the rise in the peaks,it is observed to have more concentration of electrons in the Fermi Energy Level.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiC was done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Thorium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation. The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Ho doped SiC.The band gap drops nearly to zero after doping with Thorium giving maximum concentration of electrons implying the change in the behaivour of Th doped SiC than the pure SiC.More number of charge carriers are present at the Fermi level.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, ChunmingNiu and ShouwuGuo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
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6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
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15. J. Lu ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

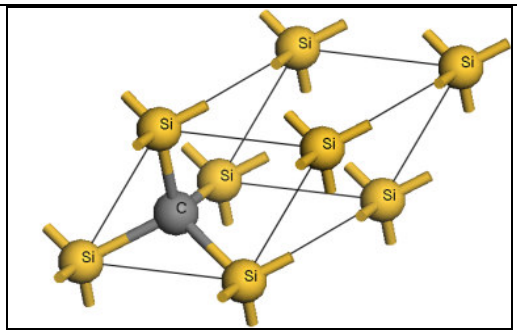

Figure 1: Crystal structure of SiC

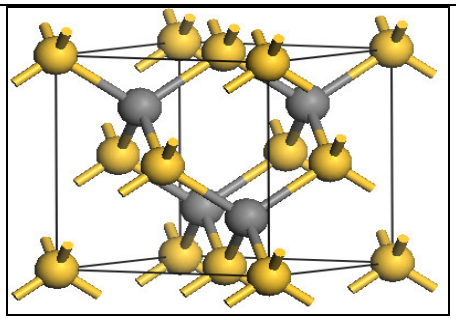

Figure.2: Primitive cell of SiC Si in yellow and C in grey.

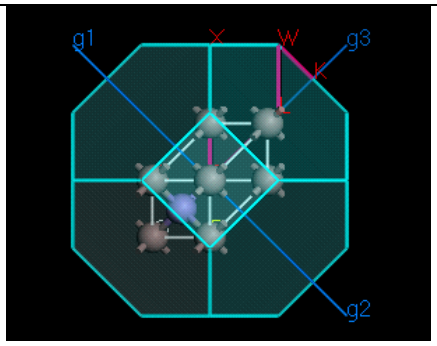

Figure 3:Brillouine zone of SiC

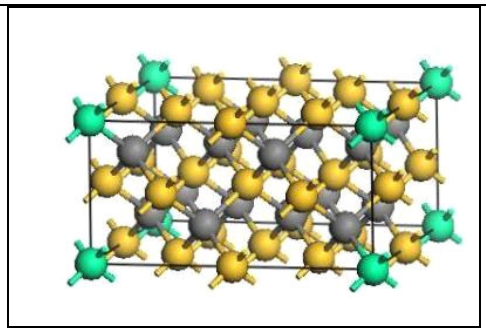

Figure 4: Thorium doped SiC supercell. Yellow color Represents Si atom,Grey is for C and green is for Kr

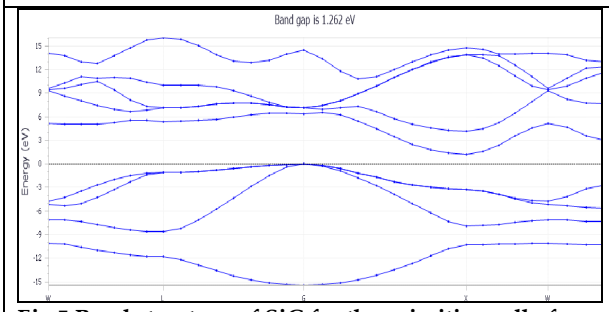

Fig 5:Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

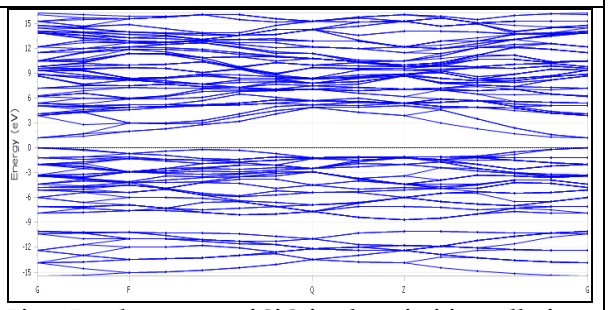

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

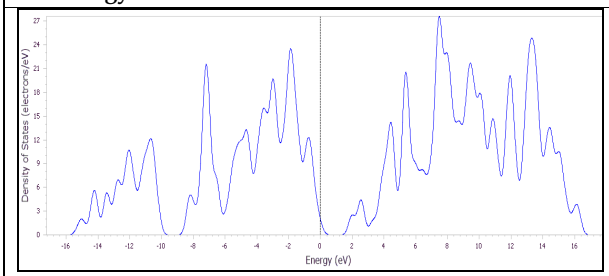

Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

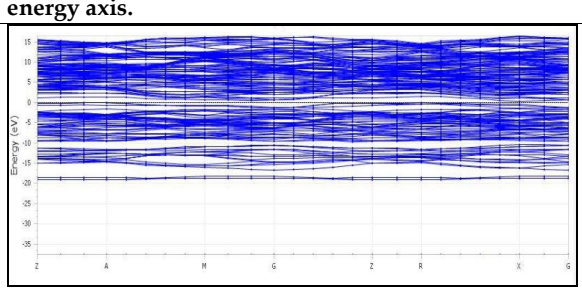

Fig 8 Band structure of Thorium dopedSiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

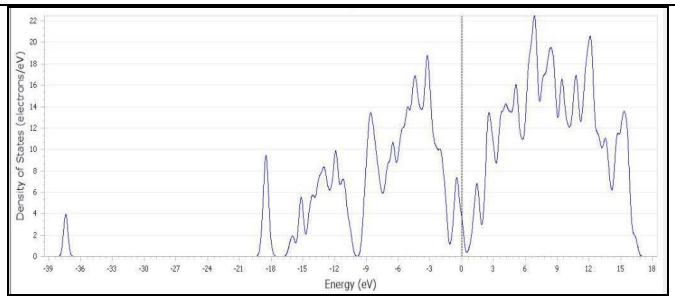

Fig 9 :Density of states of Titanium dopedSiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

First Principle Calculations of Electronic Properties of Ruthenium Doped Silicon Carbide

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ABSTRACT

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Keywords: frequency, work, structure, parameters, electrical, Ruthenium, energies

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap

semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN(3.4)eV), diamond (5.5eV),ZnS(3.6eV) etc.Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC,GaN and ZnOetc.) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties. Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high-power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2].Its properties have made SiC a research focus till date [3,4,5]. This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC. Then, SiC was doped with Ruthenium and the changes after adding the impurity was observed by comparing the undoped and doped results. The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials[6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger [8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels.The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Ruthenium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Ruthenium atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undoped SiC and doped SiC with Ruthenium are compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubiccrystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is shown inFig.2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in the form 2x2x1in X-, Y- and Z-direction. The corner Silicon atom is replaced with Ruthenium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Ruthenium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undoped SiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 8 shows the band energy plot for SiC doped with Ruthenium in the supercell calculation. Comparing with the energy bands shown in Fig. 6 it is observed that the band gap decreased after doping with Ruthenium. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence and conduction band is more towards the both sides of bandgap.

Fig. 9 shows the DOS plot for SiC doped with Ruthenium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that there is noband gapafter doping with Ruthenium near fermi energy level. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence has changed. Maximum number of charge have gathered at the top of the band and the lower portion of the valence band is less populated.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Ruthenium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observationscan be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Ru doped SiC. The band gap remains the same before and after doping with Ruthenium. But the indirect band gap of SiC has now changed to direct band gap. This indicates a change in the behavior of Rudoped SiC than pure SiC.We observed that there is no band gap after doping with Ruthenium. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence and conduction band is more towards the both sides of bandgap. It may show metallic property as well semiconductor property.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).

15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

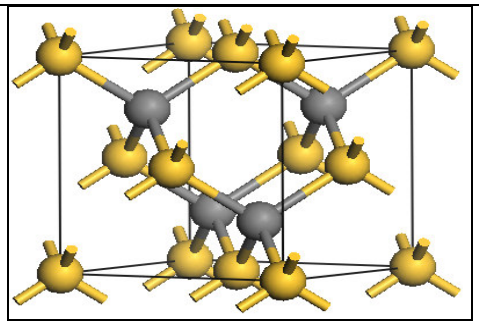

Figure 1: Crystal structure of SiC

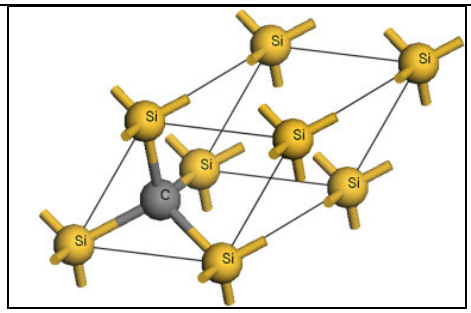

Figure 2: Primitive cell of SiC Si in yellow and C in grey.

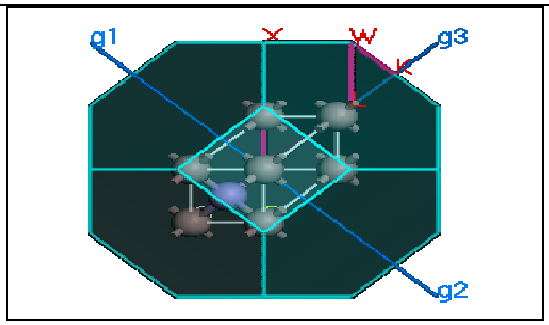

Figure .3:Brillouine zone of SiC

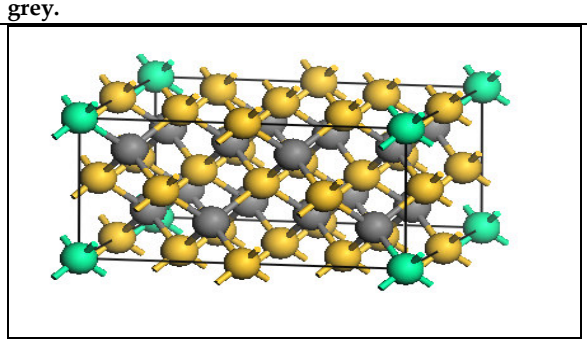

Figure 4: Ruthenium doped SiC supercell.Yellow color represents Si atom, Grey is for C atoms and Pink is for Ruthenium atoms.

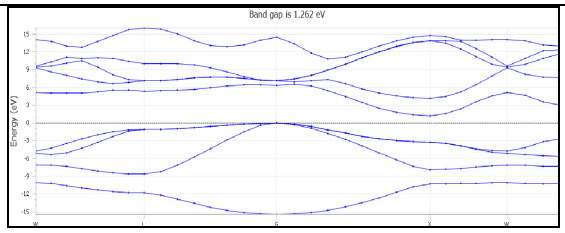

Fig 5:Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

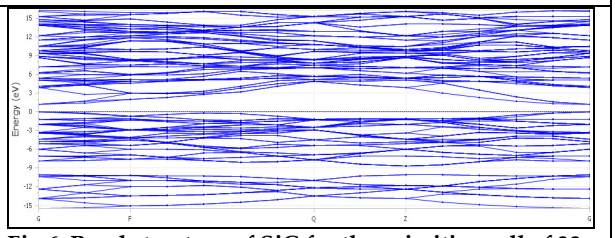

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

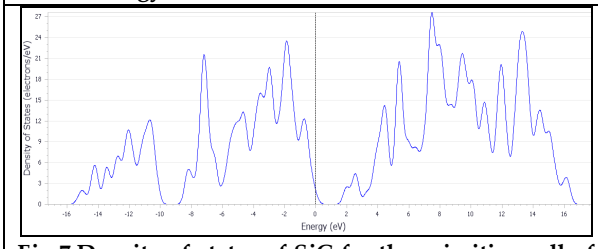

Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

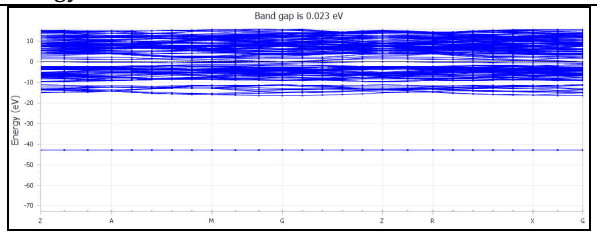

Fig 8: Band structure of Ruthenium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

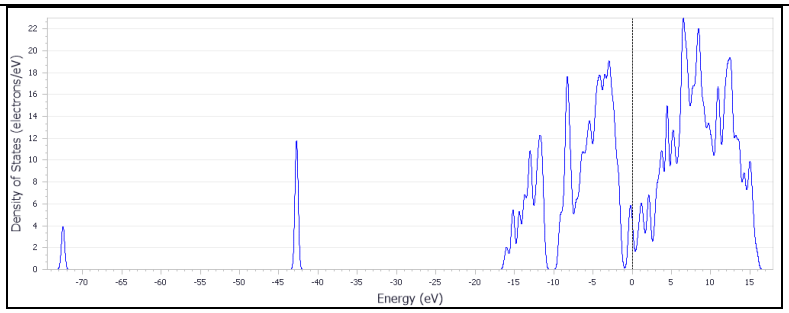

Fig 9 Density of states of Ruthenium dopedSiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy

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RESEARCH ARTICLE

First Principle Verification Electronic Properties of Rhodium Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties likehighspeed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Rhodium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Rhodium doping on SiC.

Keywords: Semiconductor, temperature, processing, Density, Rhodium

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp.

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RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

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CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Rhodium. The calculations were done using the Dassault system BIOVIA-Material Studio.Our observations can be summarized as follows. The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Rh doped SiC. DOS plot for SiC doped with Rhodium in the supercell calculation shows band gap vanished which indicate that when Rhodium doped with SiC it may show metallic property than semi-conductor property. However this cannot be confirmed without doing spin polarized calculations.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

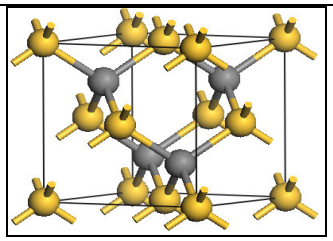

Figure 1: Crystal structure of SiC

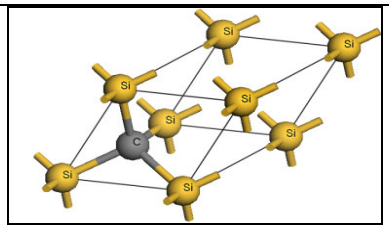

Figure 2: Primitive cell of SiC Si in yellow and C in grey.

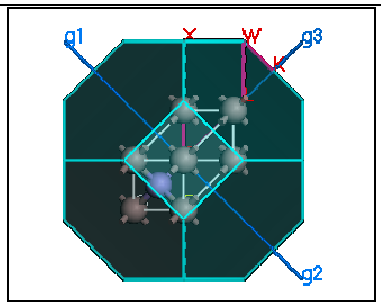

Figure 3: Brillouine zone of SiC

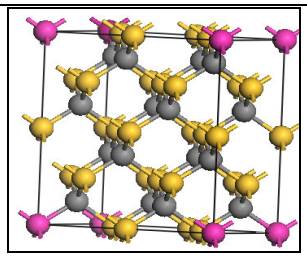

Figure 4: Rhodium doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Pink is for Rhodium atoms.

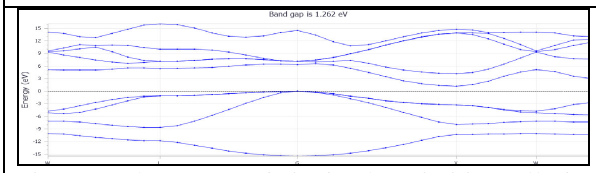

Fig 5 : Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

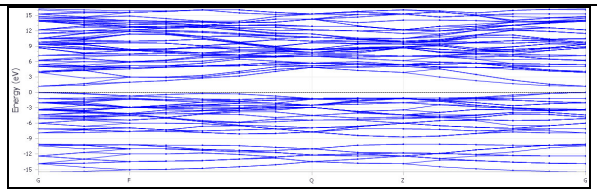

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

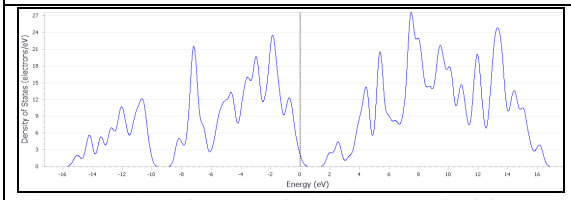

Fig 7 Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

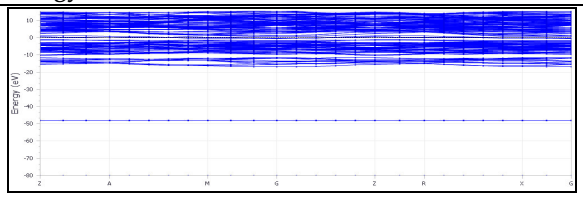

Fig 8: Band structure of Rhodium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

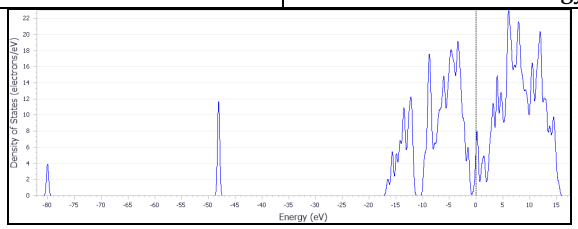

Fig 9. Density of states of Titanium dopedSiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

First Principle Verification Properties of Krypton Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like high speed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Krypton and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Krypton doping on SiC.

Keywords: SiC, parameters, Density, structure, Krypton

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC (band gap:2.3 to 3.4 eV), GaN (3.4)eV), diamond (5.5eV), ZnS (3.6eV) etc.

Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC, GaN and ZnOetc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8 V/m for different polytypes), high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high power devices to operate in higher value of blocking voltage. High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5]. This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC. Then, SiC was doped with Krypton and the changes after adding the impurity was observed by comparing the undoped and doped results. The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials [6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger [8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels. The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Krypton in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Krypton atom is placed in place of Si atom. So the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell.

The band energies, band plot and the density of states of undopedSiC and doped SiC with Krypton are compared and presented here. The calculations for the structural properties of the SiC was done taking a face centered cubic crystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is shown in Fig. 2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in the form 2x2x1 in X-, Y- and Z-direction. The corner Silicon atom is replaced with Krypton atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Krypton atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiC were done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis. The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating an indirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA. Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell. More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undopedSiC using first principle DFT with LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 8 shows the band energy plot for SiC doped with Krypton in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that there is no gap between the valence and conduction bands after SiC is doped with Krypton. Fig. 9 shows the DOS plot for SiC doped with Krypton in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the band gap of SiC vanishes after begin doped with Krypton. Small peaks are seen inside the band gap region. The Fermi level has shifted up. That indicates the increase in the highest occupied energy level. This may be an indication of the electronic properties changing from semiconductor towards metal.

CONCLUSIONS

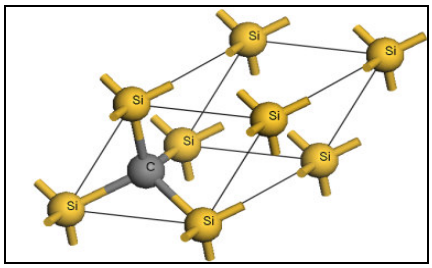
The first principle DFT calculations to study the structural and electronic properties of cubic SiC was done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiCdoped with Krypton. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation. The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Ho doped SiC.The band gap decreases to zero after doping with Krypton.Small peaks are seen inside the band gap region. The Fermi level has shifted up. That indicates the increase in the highest occupied energy level. This may be an indication of the electronic properties changing from semiconductor towards metal.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A. R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, ChunmingNiu and ShouwuGuo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)

14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999



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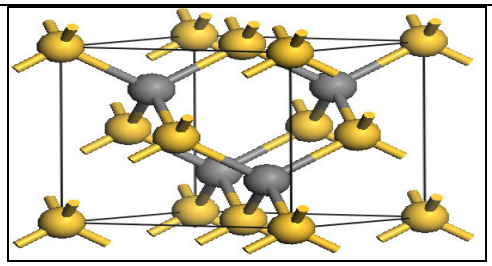


Figure .2: Primitive cell of SiC Si in yellow and C in grey.

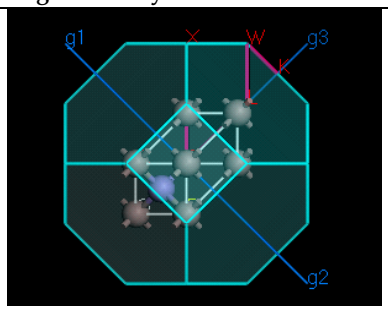


Figure 3: Brillouine zone of SiC

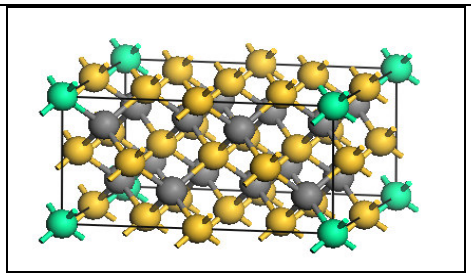


Figure 4: Krypton doped SiC supercell. Yellow color Represents Si atom,Grey is for C and green is for Kr

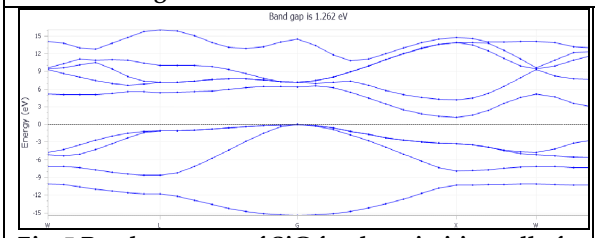
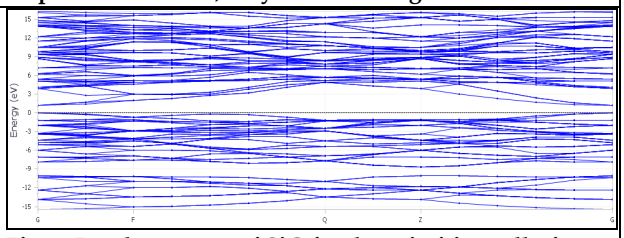


Fig 5.Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.



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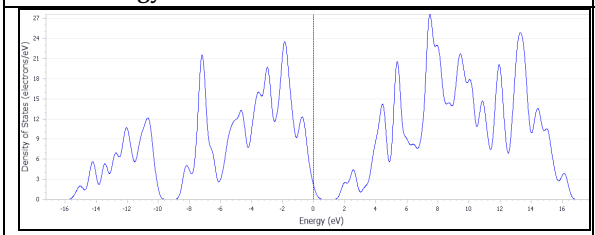


Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

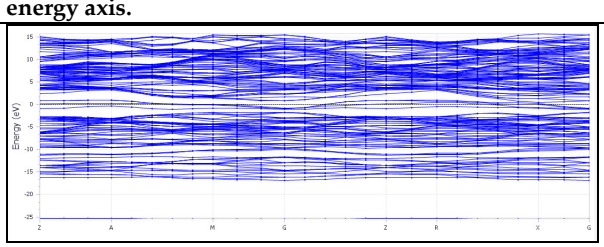
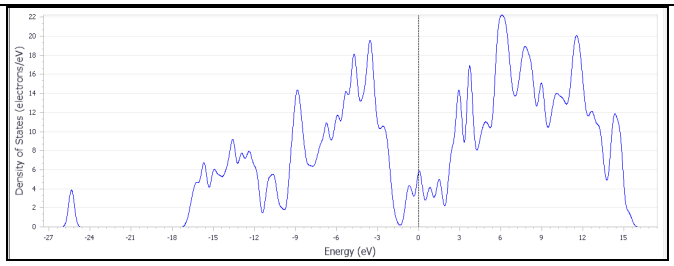


Fig 8: Band structure of Krypton dopedSiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.



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RESEARCH ARTICLE

Lanthanum Doped Silicon Carbide – A Computational Approach

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Keywords: Theory, Lanthanum, parameters, structure, temperature

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The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger [8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels. The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping with Lanthanum in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Boron atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undoped SiC and doped SiC with Lanthanum are compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubic crystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is

shown in Fig. 2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in the form 2x2x1 in X-, Y- and Z-direction. The corner Silicon atom is replaced with Lanthanum atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Boron atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTSANDDISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiC were done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis. The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell. More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undoped SiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV.

Fig. 8 shows the band energy plot for SiC doped with Lanthanum in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that the band gap remains the same before and after doping with Lanthanum. Most of the electrons have on both sides of the band gap region.Fig. 9 shows the DOS plot for SiC doped with Lanthanum in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the band gap vanishes after doping with Lanthanum. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence and conduction band is also same in both undoped and doped cases.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiC was done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Lanthanum. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for La doped SiC. The band gap vanishes after doping with Lanthanum .

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A. R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

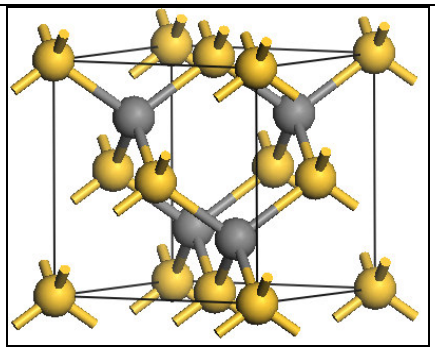


Figure 1: Crystal structure of SiC

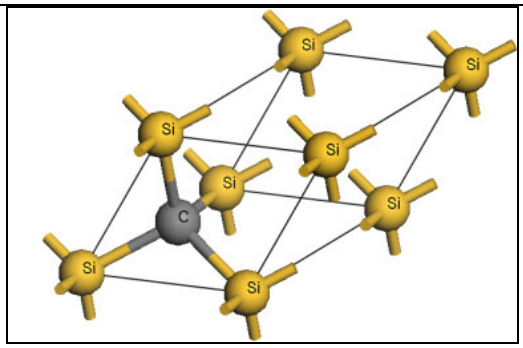


Figure 2: Primitive cell of SiC Si in yellow and C in grey.

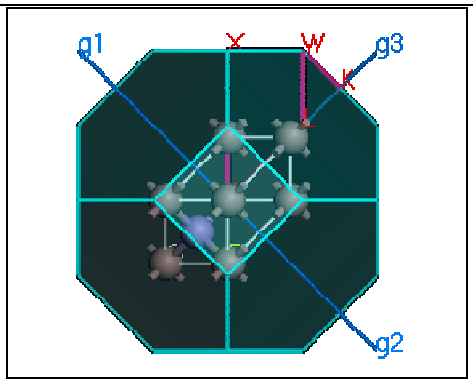


Figure 3:Brillouine zone of SiC

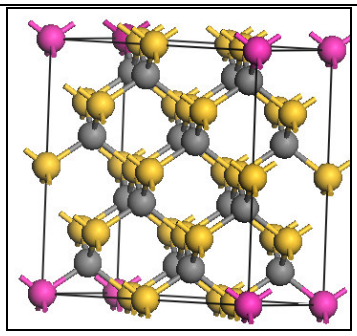


Figure 4: Lanthanum doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Pink is for Lanthanum atoms.

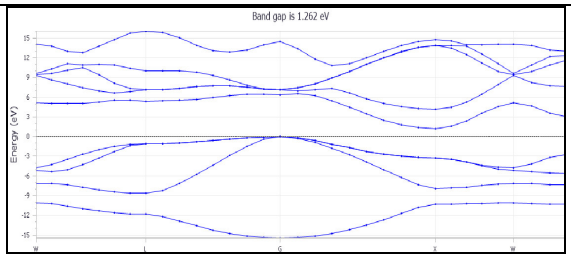


Fig 5 :Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

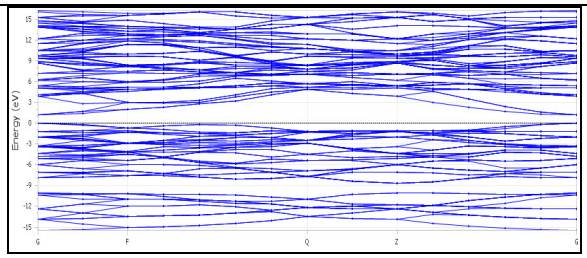


Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

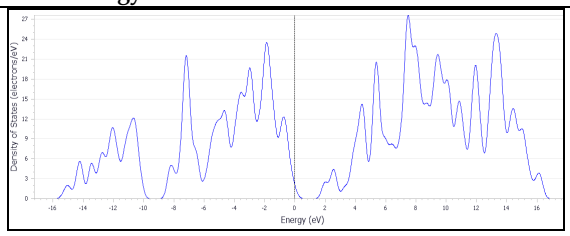


Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

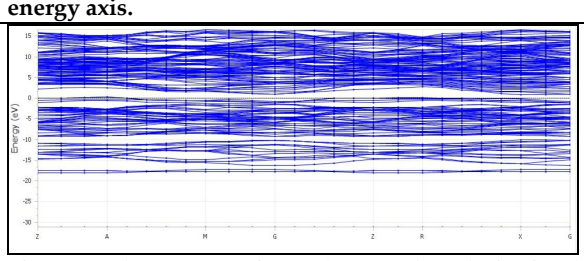
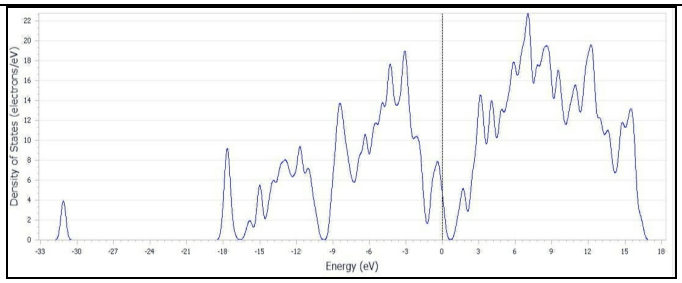


Fig 8: Band structure of Lanthanum doped SiC for the primitive cell of 32 atoms. Top of the valence bandis taken as zero on the energy axis.



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RESEARCH ARTICLE

Molybdenum Doped Silicon Carbide – A Density Functional Theory Approach

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like high speed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Molybdenum and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Molybdenum doping on SiC.

Keywords: temperature, structure, Molybdenum, SiC, bandgap

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap

semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN(3.4)eV), diamond (5.5eV),ZnS(3.6eV) etc.Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC,GaN and ZnOetc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8 V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiCcrystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC,can enable the high power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5]. This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC.Then, SiC was doped with Molybdenum and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials [6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work.Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

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CONCLUSIONS

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REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, ChunmingNiu and ShouwuGuo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
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6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn,Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
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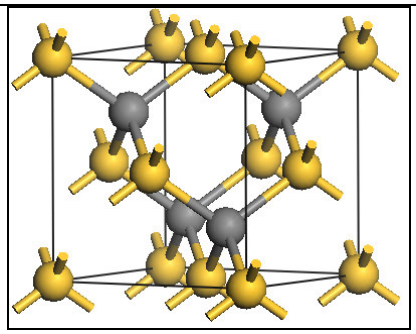

Figure 1: Crystal structure of SiC

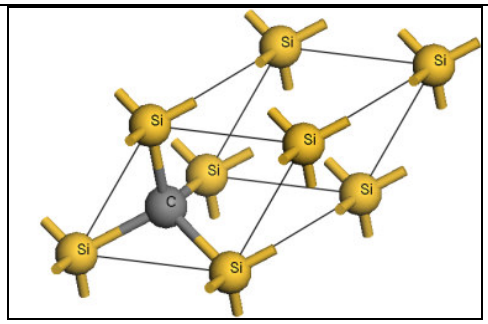

Figure 2: Primitive cell of SiC Si in yellow and C in grey.

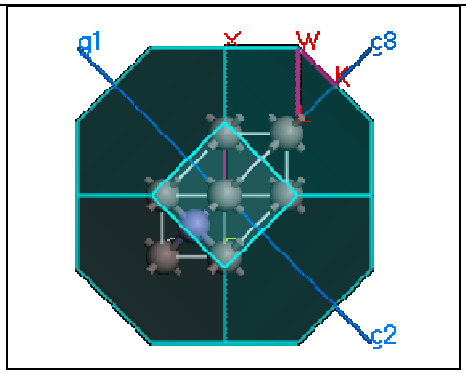

Figure 3:Brillouine zone of SiC

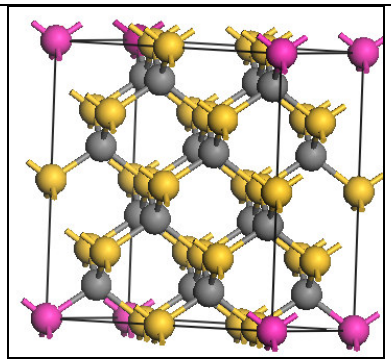

Figure 4: Boron doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Pink is for Molybdenum atoms.

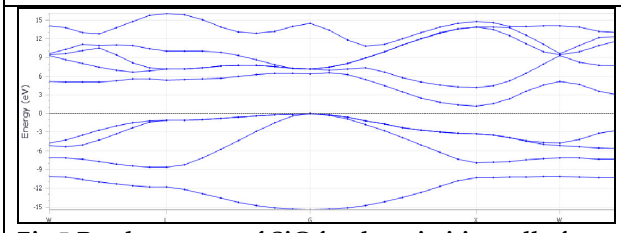

Fig 5 Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

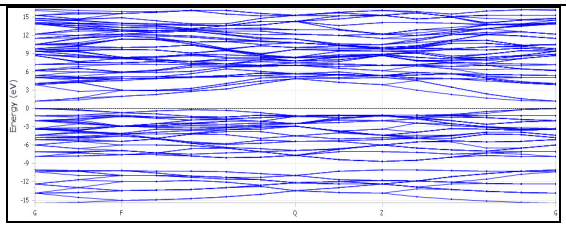

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

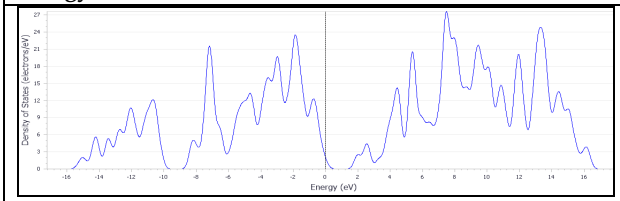

Fig 7: Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

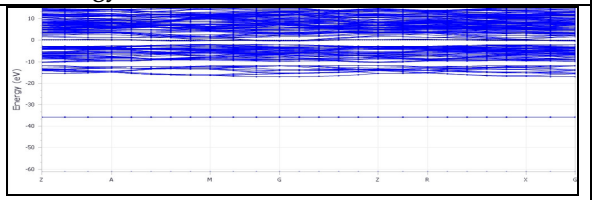

Fig 8: Band structure of Molybdenum doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

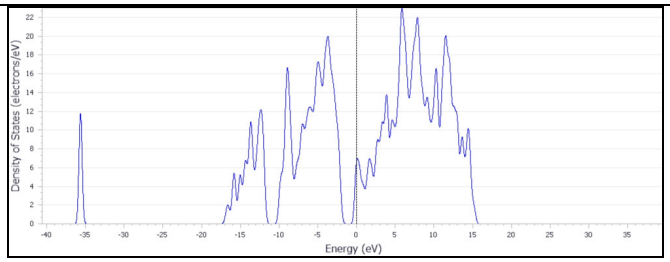

Fig 9 :Density of states of Molybdenum doped SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Palladium Doped Silicon Carbide– A Computational Approach

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like highspeed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Palladium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Palladium doping on SiC.

Keywords: highspeed, Density, electrical, parameters, Palladium, doping

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN(3.4)eV), diamond (5.5eV),ZnS(3.6eV) etc.Silicon has ruled the electronics industry since its beginning.

But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC,GaN and ZnOetc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^{8}V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiCcrystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC,can enable the high power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5]. This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC.Then, SiC was doped with Palladium and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials[6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work.Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger[8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels.The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Palladium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Palladium atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undopedSiC and doped SiC with Palladiumare compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubiccrystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is

shown inFig. .2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in the form 2x2x1in X-, Y- and Z-direction. The corner Silicon atom is replaced with Palladium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Palladium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTSANDDISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort.

The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap. The total density of states (DOS) of undopedSiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 8 shows the band energy plot for SiC doped with Palladium in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that the band gap becomes zero after doping with Palladium. This indicates a change in the conductivity ofPddoped SiC than pure SiC. Fig. 9 shows the DOS plot for SiC doped with Palladium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that small peaks are seen inside the band gap after doping with Palladium. The Fermi level is seen between the valence and conduction band. The lower portion of the valence band is less populated in comparison to undoped SiC.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC.All these were also done for SiC doped with Palladium. The calculations were done using the Dassault system BIOVIA-Material Studio.Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Pddoped SiC. The band gap disappears doping with Palladium and conductivity may change due to this. This indicates a change in the behavior of Pddoped SiC than pure SiC.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, ChunmingNiu and ShouwuGuo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn,Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

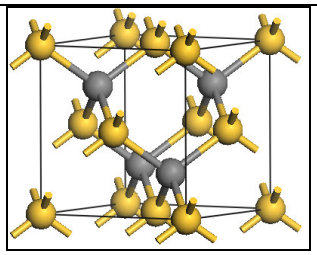


Figure 1: Crystal structure of SiC

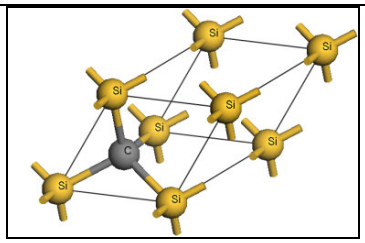


Figure 2: Primitive cell of SiC Si in yellow and C in grey.

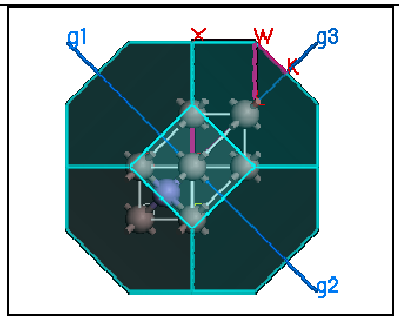


Figure 3:Brillouine zone of SiC

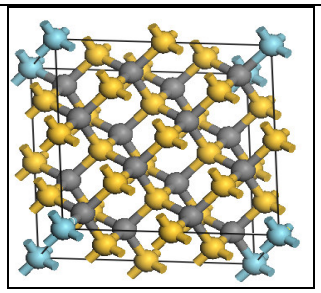


Figure 4: Palladium doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and blue is for Palladium atoms.

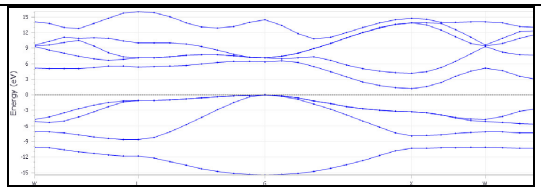
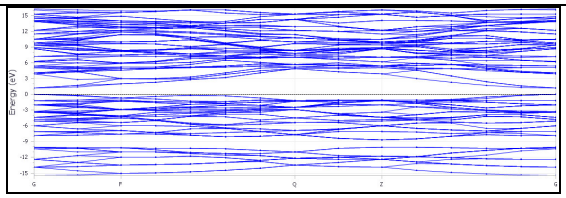


Fig 5: Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.



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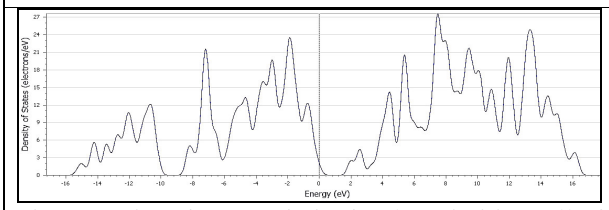


Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

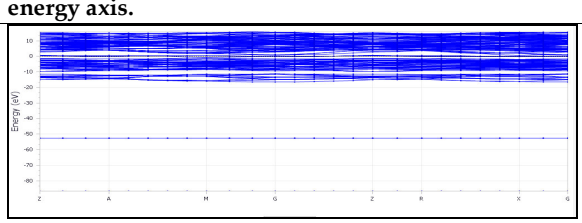
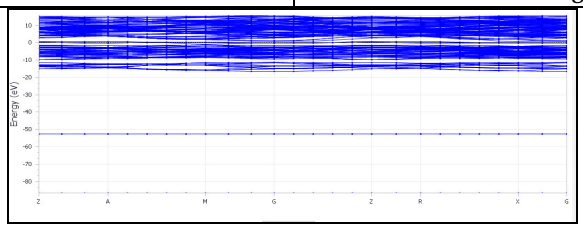


Fig 8: Band structure of Palladium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.



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RESEARCH ARTICLE

Properties of Actinium Doped Silicon Carbide– A Density Functional Theory

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ABSTRACT

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Keywords: density, Semiconductor, Actinium, structure, energies

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Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

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We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5 The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undoped SiCusing first principle DFTwith LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 8 shows the band energy plot for SiC doped with Actinium in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that the band gap remains the same before and after doping with Actinium. But the indirect band gap of SiC has now changed to direct band gap. This indicates a change in the behavior ofAc doped SiC than pure SiC. Fig. 9 shows the DOS plot for SiC doped with Actinium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the band gap becomes zero after doping with Actinium. DOS curves are continuous from valence band to conduction band. Fermi level has moved a little up in energy indicating increase value of highest occupied energy level. Small peaks inside the band gap shows presence of charge carriers inside this portion. The DOS plot show many peaks but it has a maximum peak at 6.0ev.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Actinium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows. The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Ac doped SiC. The band gap decreases to zero after doping with Actinium and it may show metallic behavior. The DOS plot show many peaks but it has a maximum peak at 6.0ev.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A.R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

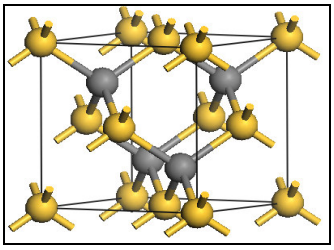

Figure 1: Crystal structure of SiC

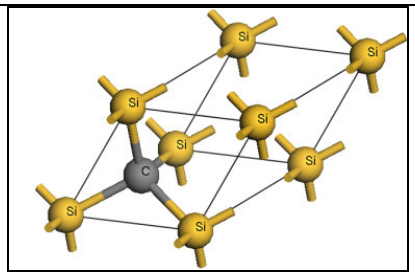

Figure 2: Primitive cell of SiC Si in yellow and C in grey.

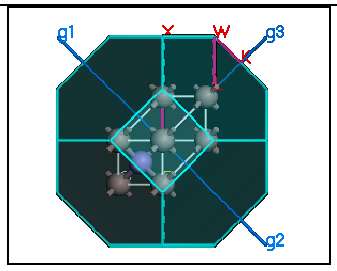

Figure 3:Brillouine zone of SiC

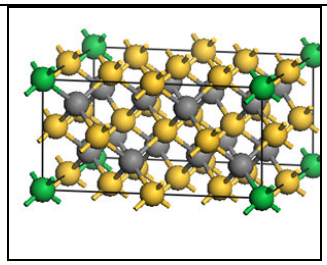

Figure 4: Actinium doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Green is for Actinium atoms.

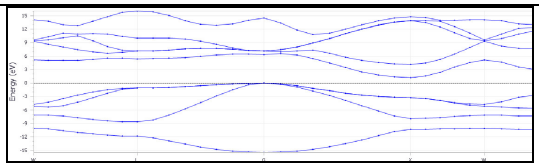

Fig 5 :Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

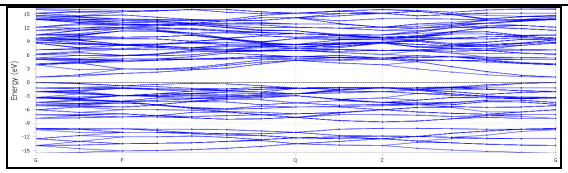

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

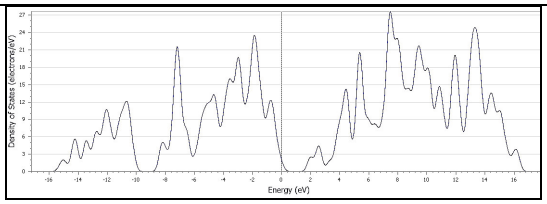

Fig 7 :Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

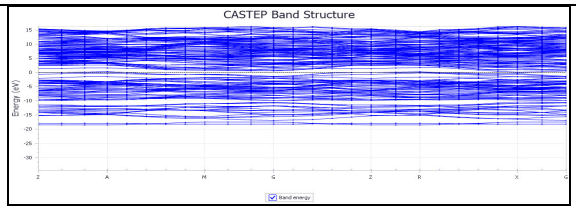

Fig 8: Band structure of Actinium dopedSiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

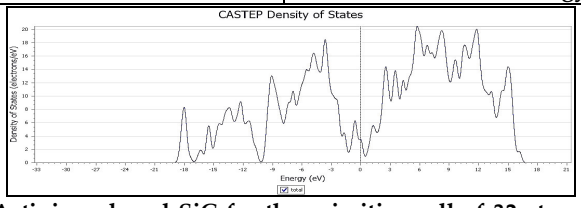

Fig 9 : Density of states of Actinium doped SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Study of the Electronic properties of Holmium Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like high speed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide band gap semiconductor has some specifically electrical properties which make it suitable for high –power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Holmium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Holmium doping on SiC.

Keywords: SiC, lattice constant, band gap, Density, Holmium

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN(3.4)eV), diamond (5.5eV),ZnS(3.6eV) etc.Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function

within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC,GaN and ZnOetc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5].This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC. Then, SiC was doped with Holmium and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials [6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger [8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels.The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Holmium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Holmium atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undoped SiC and doped SiC with Holmium are compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubiccrystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is shown inFig 2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in the form 2x2x1in X-, Y- and Z-direction. The corner Silicon atom is replaced with Holmium atom. The new primitive

cell contains total 32 atoms with 15 Silicon atoms, 1 Holmiumatom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

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We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig.6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

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CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiC were done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Holmium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation. The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Holmium doped SiC. Electron concentration more both side of the Fermi energy level in Ho doped SiC compared to pure SiC.DOS plot shows band gap decreases when SiC doped with Holmium.DOS plot of Holmium doped SiC shows a high peak at Fermi energy level.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A. R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
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6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
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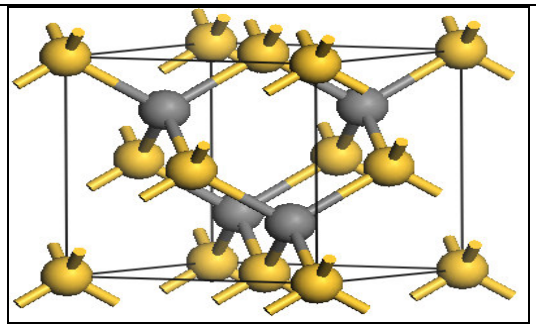

Figure 1: Crystal structure of SiC

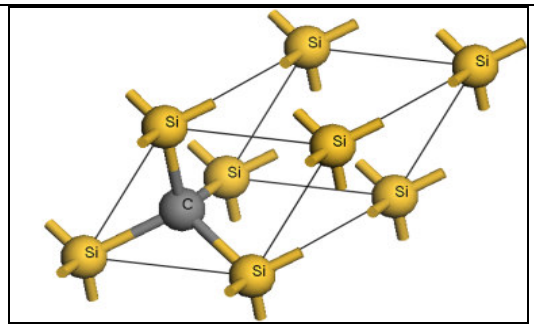

Figure 2: Primitive cell of SiC
Si in yellow and C in grey.

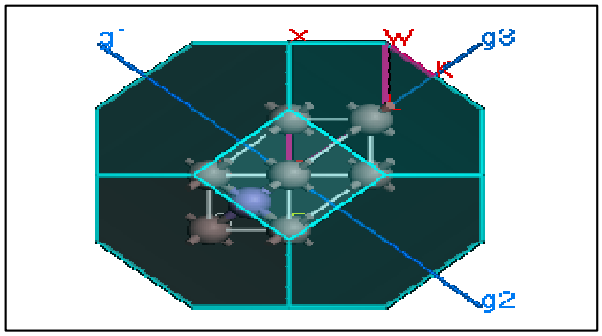

Figure 3: Brillouine zone of SiC

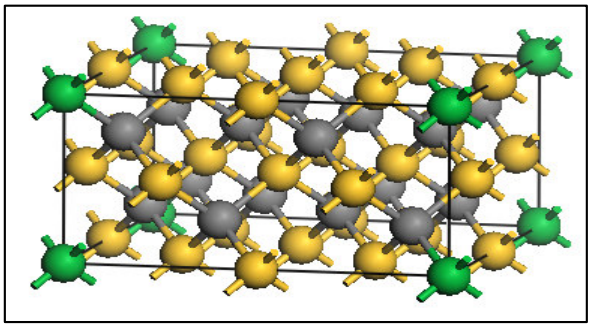

Figure 4:Holmium doped SiC supercell.
Yellow color represents Si atom, Grey is for C atoms and Green is for Holmium atoms.

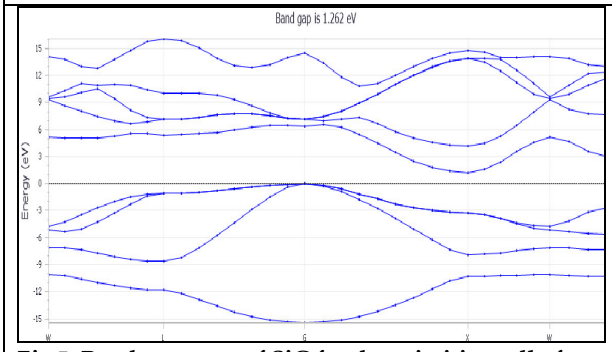

Fig 5: Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

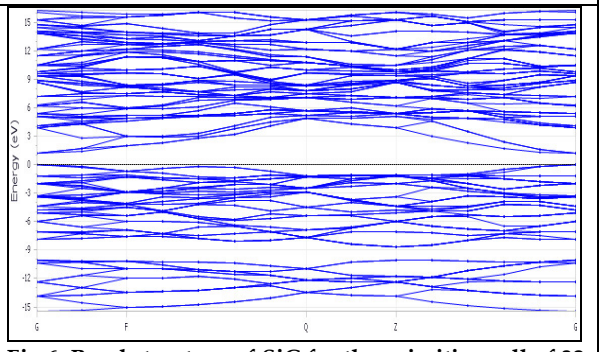

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

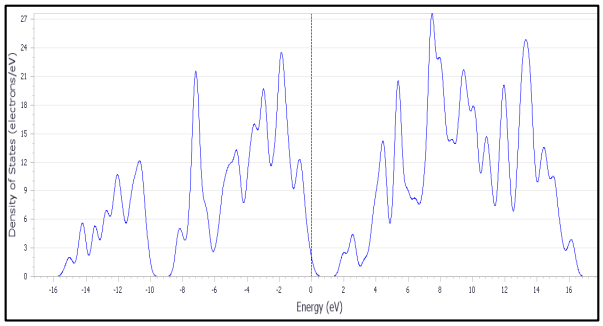

Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

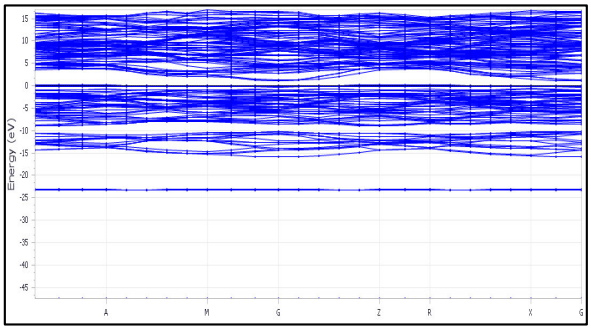

Fig 8: Band structure of Holmiumdoped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

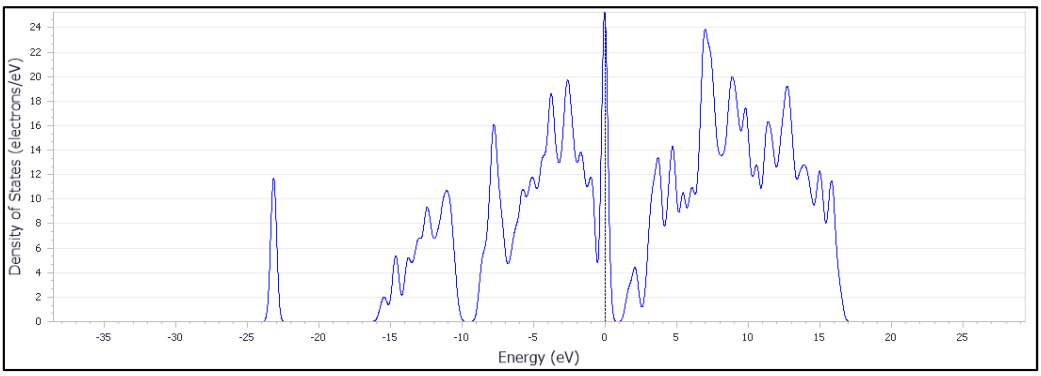

Fig 9: Density of states of Holmium doped SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

Studying the Electronic Properties of Cadmium Doped Silicon Carbide with Density Functional Theory

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties likehighspeed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide bandgap semiconductor has some specifically electrical properties which make it suitable for high – power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Cadmium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Cadmium doping on SiC.

Keywords: Cadmium Doped, Silicon Carbide, Density, Functional Theory, band energies

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is

not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC(band gap:2.3 to 3.4 eV),GaN (3.4)eV), diamond (5.5eV),ZnS (3.6eV) etc. Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC, GaN and ZnO etc) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties . Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC,can enable the high power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2]. It properties has made SiC a research focus till date [3,4,5].

This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC.Then, SiC was doped with Cadmium and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials [6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger[8] parametrization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels.The zinc blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Cadmium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Cadmium atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undoped SiC and doped SiC with Cadmium

are compared and presented here. The calculations for the structural properties of the SiC was done taking a face centered cubiccrystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is shown inFig. 2 and the BZ sampling is shown in Fig. .3. A supercell was created by expanding the lattice constant in the form 2x2x1in X-, Y- and Z-direction. The corner Silicon atom is replaced with Cadmium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Cadmium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort.

The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of un doped SiC using first principle DFT with LDA using pseudo potential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig.8 shows the band energy plot for SiC doped with Cadmium in the supercell calculation. Comparing with the energy bands shown in Fig. 6, it is observed that the band gap betweeconduction band and valence band vanishes giving a zero band gap after doping. This may indicates a better conductivity behavior of Cd doped SiC. Fig. 9 shows the DOS plot for SiC doped with Cadmium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the band gap does not exist after doping with Cadmium and the DOS plot is now continuous.The distribution of electrons in the valence and conduction band also changes in both undoped and doped cases. It can be clearly seen that most of the charge carriers have gathered at the boundary line between valence and conduction band.

CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC.All these were also done for SiC doped with Cadmium. The calculations were done using the Dassault system BIOVIA-Material Studio.Our observations can be summarized as follows. The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Cddoped SiC. The band gap vanishes after doping with Cadmium. This may indicates the improved conductivity ofCd doped SiC than pure SiC.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A. R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, ChunmingNiu and ShouwuGuo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn,Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

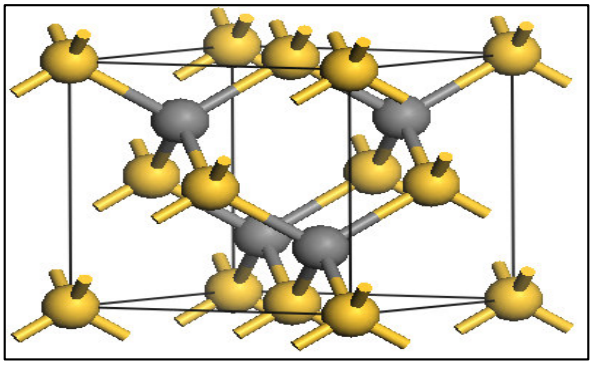


Figure 1: Crystal structure of SiC (Si in yellow and C in grey)

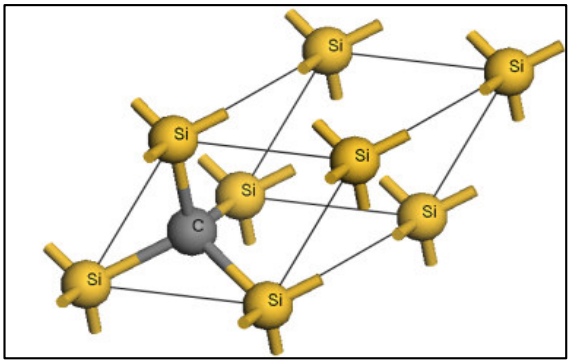
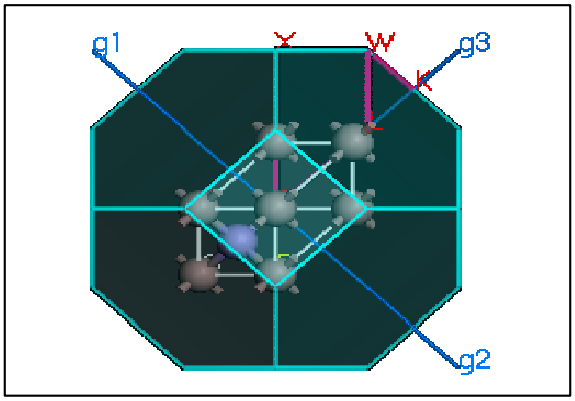


Figure 2: Primitive cell of SiC (Si in yellow and C in grey)



. **Figure 3:Brillouine zone of SiC**

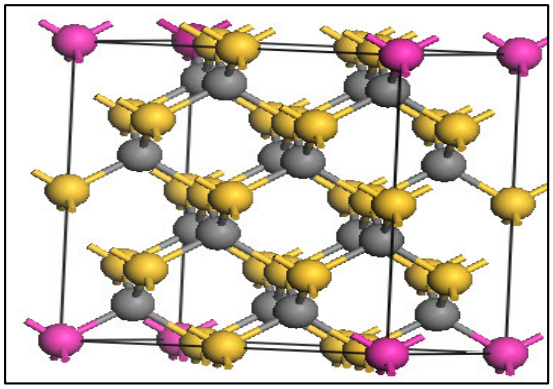


Figure 4:Cadmium doped SiC supercell.

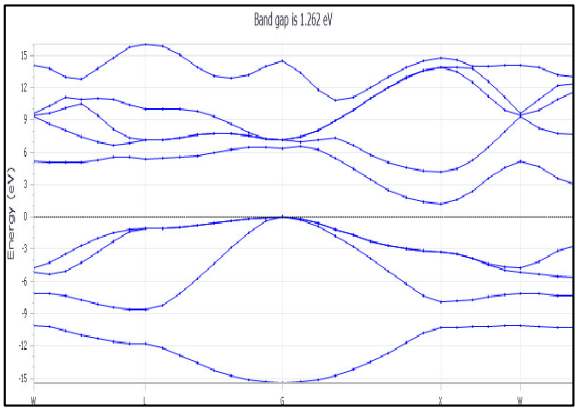


Fig 5 :Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

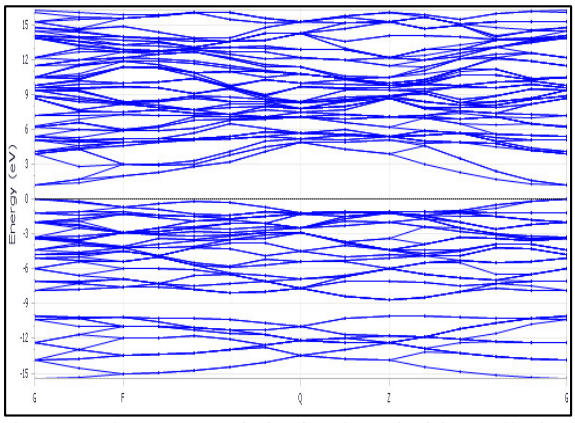


Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

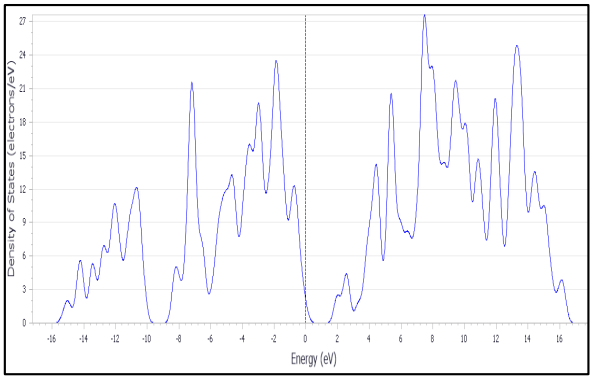


Fig 7 :Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

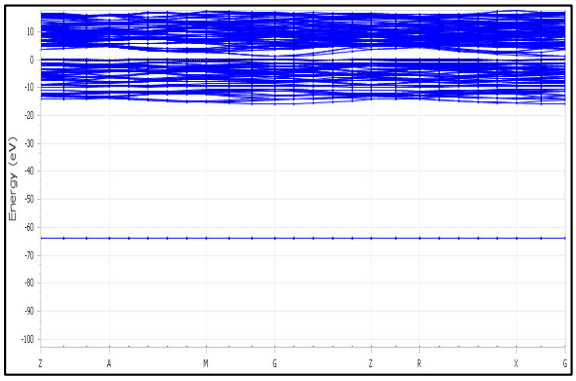
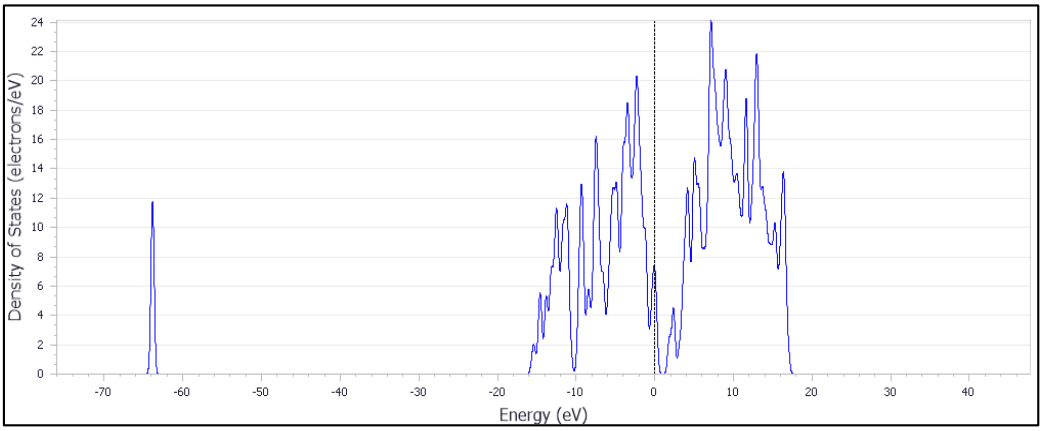


Fig 8: Band structure of Cadmium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.



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RESEARCH ARTICLE

Studying Zirconium Doped Silicon Carbide Computationally

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ABSTRACT

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Keywords: Zirconium Doped, Silicon Carbide, Density, lattice constant

INTRODUCTION

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RESULTS AND DISCUSSIONS

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Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A^{o}. The experimental lattice constant value for SiC is 4.359A^{o}. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort. The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating anindirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell. More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

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CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiCwas done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Zirconium. The calculations were done using the Dassault system BIOVIA-Material Studio.Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745A^{o}. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation.The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Zr doped SiC. The band gap energy for Zr doped Sic is found to be 1.604eV. Due to the doping of Zirconium, the band gap between CB and VB of SiC increases. The increase in bandgap may result in fewer electrons moving from the CB to the VB, resulting in a noticeable decrease in the interaction between electrons. Hence the conductivity of SiC decreases with doping of Zr.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A. R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

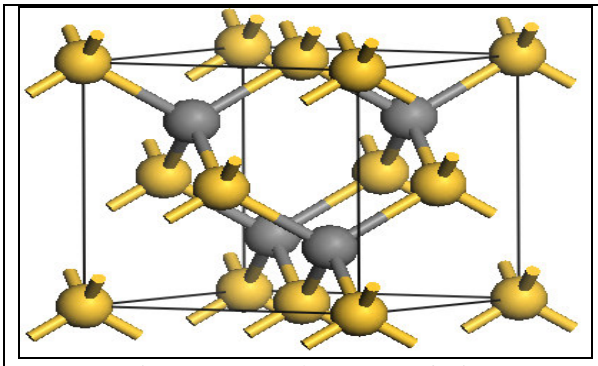

Figure 1: Crystal structure of SiC

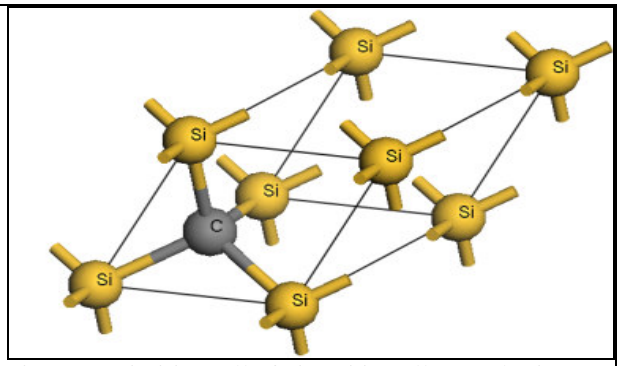

Figure 2: Primitive cell of SiC Si in yellow and C in grey

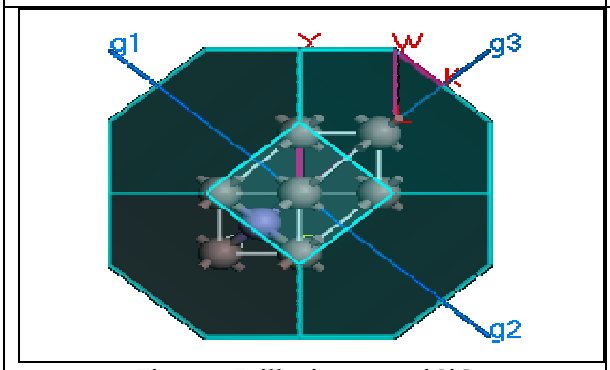

Figure 3: Brillouine zone of SiC

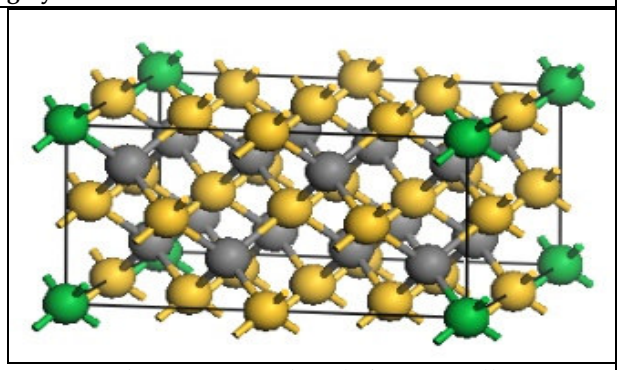

Figure 4: Boron doped SiC supercell
Yellow color represents Si atom, Grey is for C atoms and Green is for Zirconium atoms

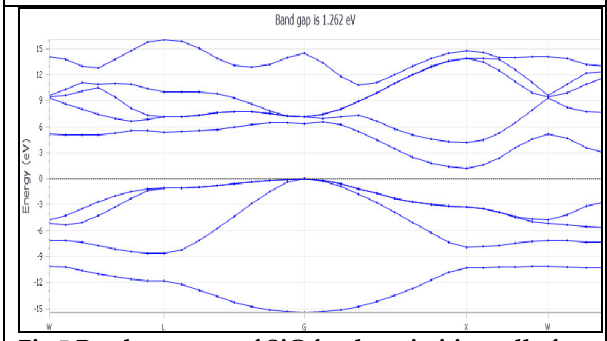

Fig 5:Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

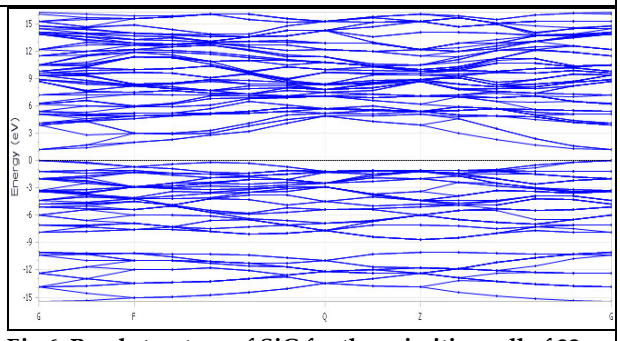

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

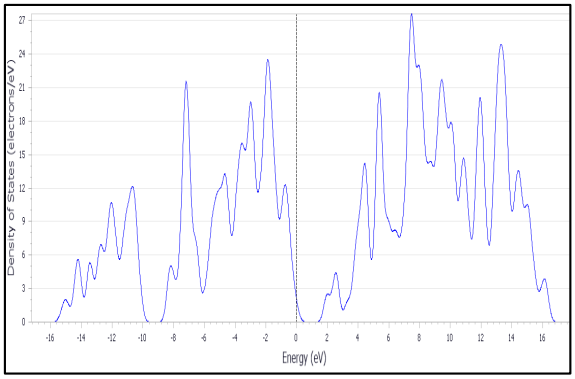

Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

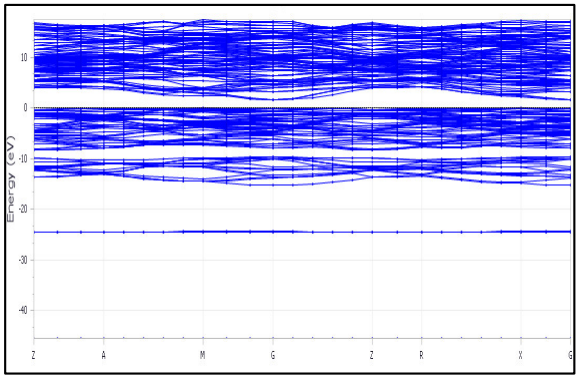

Fig 8: Band structure of Zirconium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

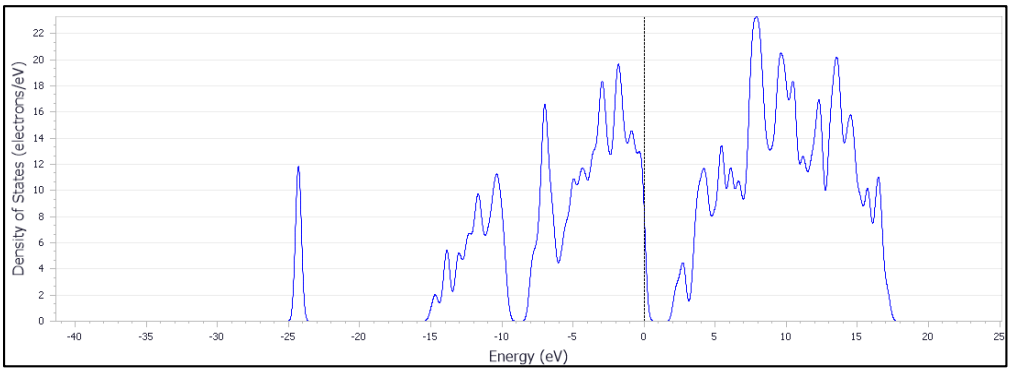

Fig 9: Density of states of Zirconium doped SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

A Computational Approach to Understand the Electronic Properties of Erbium Doped Silicon Carbide

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like high speed, simple processing, useful temperature range etc. The most suitable quality is that they can be doped with some impurities to modify their properties in a controlled manner. SiC which is a wide band gap semiconductor has some specifically electrical properties which make it suitable for high –power and high- frequency uses. It is important to understand the properties of SiC for its use in electronics devices. Using the first principle Density Functional Theory, different parameters like lattice constant, band gap, band plot and density of states are calculated in this work. . The band structure calculation was done, plotted and the band gap was found out. SiC was doped with Erbium and the band energies were calculated. Plotted the band structure with the impurity and also plotted the Density of states. The results obtained before and after doping were compared to find the effect of Erbium doping on SiC.

Keywords: Erbium Doped, Silicon Carbide, Density, band gap, lattice constant

INTRODUCTION

Semiconductor materials have been playing a crucial role in the electronics industry. They are especially important as varying conditions like temperature and impurity content can easily change their conductivity. Semiconductors are mainly classified according to their electrical conductivity and band gap. At very low temperature a semiconductor behaves as an insulator but shows good conductivity at room temperature. Materials with band gap less than 3 eV are generally semiconductors and with band gap more than 3 eV are insulators. However, the limit is not very sharp. Semiconductors with band gap towards or even more than the higher limit are called wide bandgap semiconductors, for example SiC(band gap:3 to 8 eV),GaN(8)eV), diamond (5.5eV),ErS(3.6eV) etc.Silicon has ruled the electronics industry since its beginning. But with the development of high speed microprocessors, shrinking size

of transistors and the increasing demand of higher efficiency electronics coupled with extreme environment operation, the limitations of silicon are new becoming prominent. Silicon based transistors can function within the temperature limit of few GHz and highly susceptible to harsh environments. On the other hand the wide bandgap semiconductors (e.g. SiC,GaN and ErOetc.) are superior to silicon due to their physical (e.g. high melting point, hardness etc.) and electrical properties. Silicon Carbide (SiC) which is a wide bandgap semiconductor has some specific electrical properties which make it suitable for high power and high frequency uses. It has high breakdown electric field (1 to 2.5×10^8V/m for different polytypes),high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes [1]. Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high-power devices to operate in higher value of blocking voltage.High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications [2].Its properties have made SiC a research focus till date [3,4,5]. This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC. Then, SiC was doped with Erbium and the changes after adding the impurity was observed by comparing the undoped and doped results.The modification in the band gap will affect or ensure the application of SiC.

Computational Method

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudo potentials[6]. The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio [7] is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Perdew and Zunger [8] parameterization of Monte Carlo calculations of Ceperley and Alder [9] method. The single particle Kohn-Sham [10] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels.The Erbium blend crystal structure of SiC [11] is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a super cell. Since we intend to do a doping of Erbium in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Erbium atom is placed in place of Si atom. SO the percentage of impurity becomes 6%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell. The band energies, band plot and the density of states of undoped SiC and doped SiC with Erbium are compared and presented here.

The calculations for the structural properties of the SiC was done taking a face centered cubic crystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is shown inFig.2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in

the form 2x2x1in X-, Y- and Z-direction. The corner Silicon atom is replaced with Erbium atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Erbium atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

RESULTS AND DISCUSSIONS

Density functional theory (DFT) [12] calculation for electronic properties of SiCwere done. SiC crystalizes in Erbium blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

Electronic Properties

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as 'zero' along the energy axis.The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort.

The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating an indirect band gap. This is in accordance with published experimental results too [13]. The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 39 eV [14]. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA.Fig. 6 shows the band plot for SiC with 32 atoms in the primitive cell.More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

The total density of states (DOS) of undoped SiCusing first principle DFTwith LDA using pseudopotential is shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot [15]. The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV. Fig. 8 shows the band energy plot for SiC doped with Erbium in the supercell calculation. Comparing with the energy bands shown in Fig. 6 it is observed that the band gap decreased after doping with Erbium.Fig. 9 shows the DOS plot for SiC doped with Erbium in the supercell calculation. Comparing with the DOS plot shown in Fig. 7 it is observed that there is a small band gap after doping with Erbium. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence and conduction band is different in both undoped and doped cases.

CONCLUSIONS

The first principle DFT calculation to study the structural and electronic properties of cubic SiC was done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Erbium. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745Ao. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation. The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for Er doped SiC. The band gap remains the same before and after doping with Erbium. But the indirect band gap of SiC has now changed to direct band gap. This indicates a change in the behavior of Er doped SiC than pure SiC. It is observed that there is a small band gap after doping with Erbium. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence and conduction band is different in both undoped and doped cases.

REFERENCES

1. Robert F. Davis, Proceedings of the International Conference in SiC and Related Materials-93, Washington DC, USA, (1993).
2. A. R. Atwell, Silicon Carbide MEMS Devices for Harse Environments, (Cornell University, 2002).
3. Dan Zhao, Xiaoyan Yuan, Beibei Li, Fan Jiang, Yi Liu, Jinying Zhang, Chunming Niu and Shouwu Guo, Silicon carbide nanowire covered by vertically oriented graphene for enhanced electromagnetic wave absorption performance, Chemical Physics, Vol. 529, January 2020, pp. 110574.
4. Naura D Alkhalidi, Sajib K Barman, Muhammad N Huda, Crystal structures and the electronic properties of silicon-rich silicon carbide materials by first principle calculations, Heliyon, Vol. 5, Issue 11, November 2019.
5. A Taylot, L Klimsa, J Kopecek, Z Remes, M Vronka, R Ctvrtlik, J Tomastik and V Mortet, Synthesis and Properties of Diamond – silicon carbide composite layers, Journal of Alloys and Compuonds, Vol. 5 September 2019, Pages 327-333
6. D. Vanderbilt, "Soft self-consistent pseudopotentials in a generalized eigenvalue formalism", Phy. Rev. B vol. 41, pp. 7892(1990).
7. N. Dahham, A. Fares, K. Najem ,Modeling and simulation of mechanical and physical properties of Barium orthotitanate, B.I.O.V.I.A, Daassault systems, Material studio, 7.0 Dassault systems , San Diego, 2017 Tikrit, J. Pure Science, 2017
8. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B vol. 23, pp 5048 (1981).
9. D. M. Ceperley and B. I. Alder, "Ground State of the Electron Gas by a Stochastic Method", Phys. Rev. Lett. vol. 45, pp 566(1980)
10. W.Kohn and I.J .Sham," Self-Consistent Equations Including Exchange and Correlation Effects", Phys.Rev.140,(1965)
11. A Taylor and D S Laidler, The Formation and Crystal Structure of Silicon Carrbide, British Journal of Applied Physics, Vol. 1, no. 7, July 1950
12. P. Hohenberg and W. Kohn, Inhomogenous Electron Gas, Physical Review B, Vol. 136, 1964, pp. 864-871
13. Bjorn Baumeier, Peter Kruger, and Johannes Pollmann, Self-interaction-corrected pseudopotentials for silicon carbide, Phys. Rev. B 73, 195205 (2006)
14. W. J. Choyke, D. R. Hamilton, and L. Patrick, Optical Properties of Cubic SiC: Luminescence of Nitrogen-Exciton Complexes, and Interband Absorption, Phys. Rev. 133, A1163 (1964).
15. J. Lu¨ning, S. Eisebitt, J.-E. Rubensson, C. Ellmers and W. Eberhardt, Electronic structure of silicon carbide polytypes studied by soft x-ray spectroscopy, Physical Review B, Vol. 15 APRIL 1999

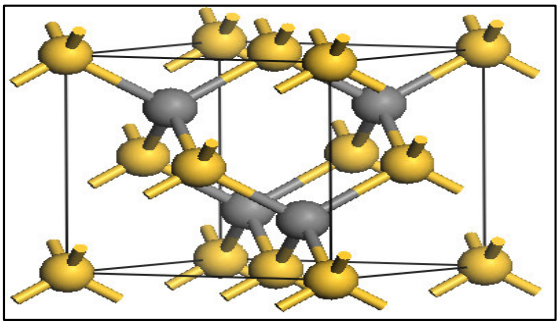

Figure 1: Crystal structure of SiC
Si in yellow and C in grey.

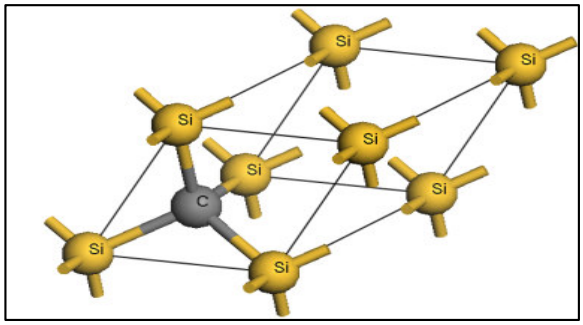

Figure 2: Primitive cell of SiC
Si in yellow and C in grey.

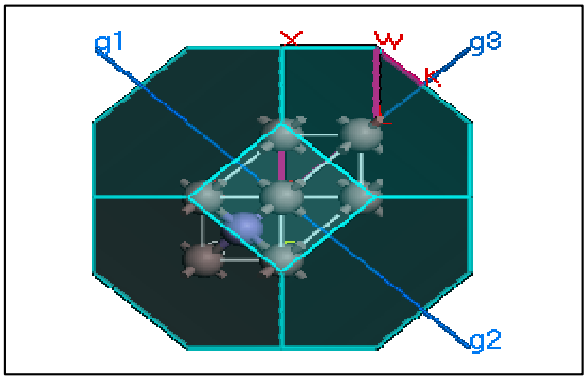

Figure3: Brillouine zone of SiC

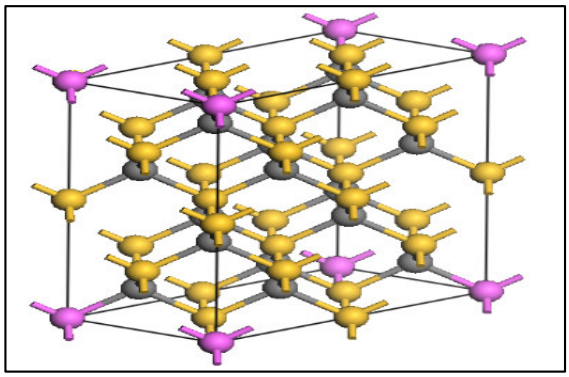

Figure 4:Erbium doped SiC supercell.
Yellow color represents Si atom, Grey is for C atoms and Pink is for Erbium atoms.

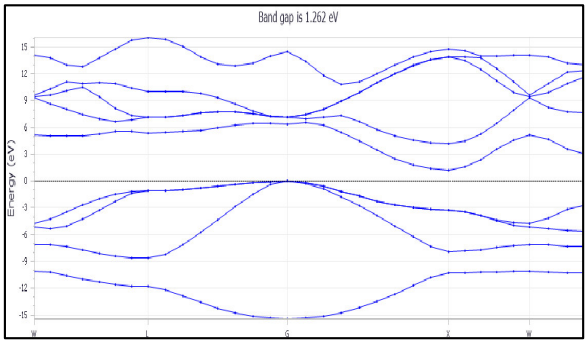

Fig 5:Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

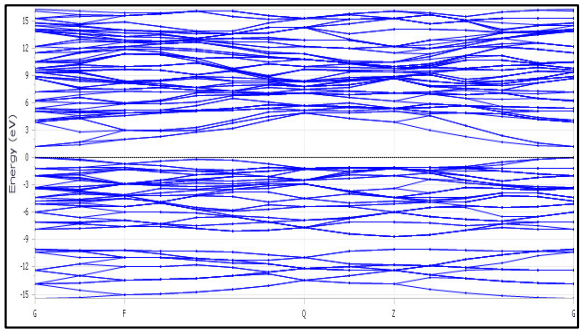

Fig 6: Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

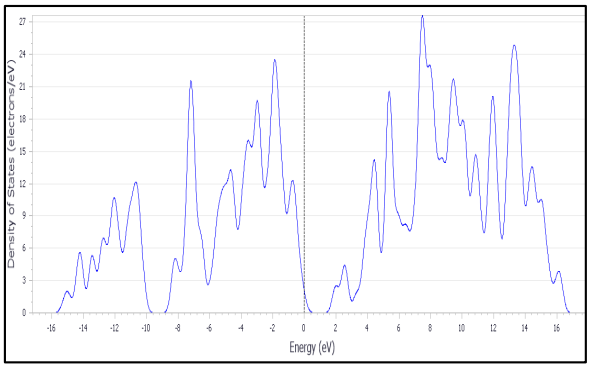

Fig 7:Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

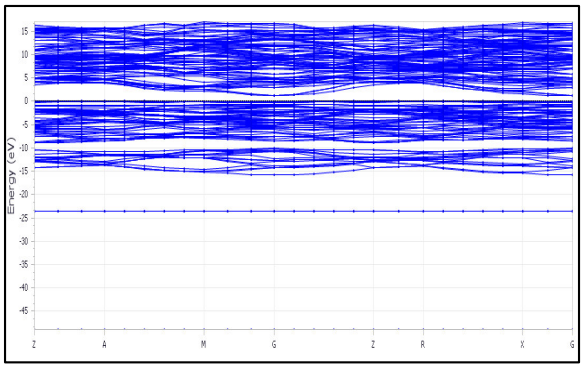

Fig 8: Band structure of Erbium doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

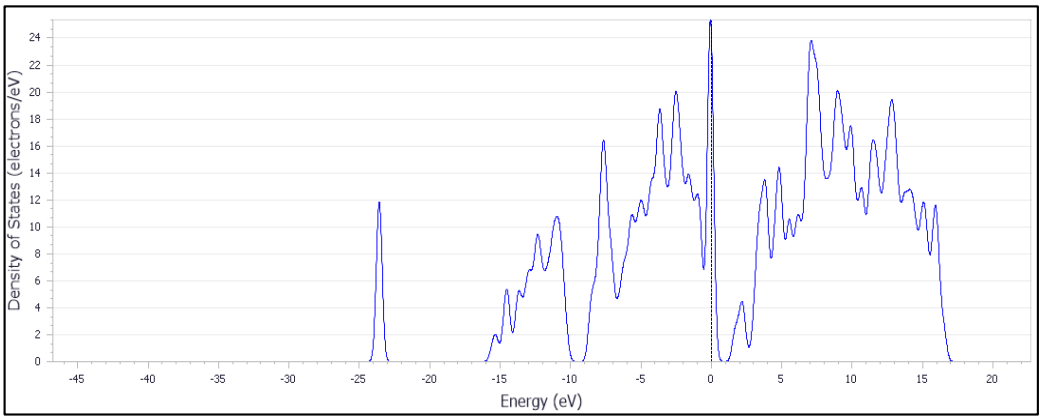

Fig 9:Density of states of Erbium doped SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

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RESEARCH ARTICLE

The Limits of the Community Empowerment Models: Case Studies from Tribal India

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ABSTRACT

India has been trying to tackle problems of poverty and under development, on a war footing. India, on independence, had debated a Gandhian, bottom-up village as center based development plan, but the then Government of India and its leadership opted for centralized planning. Five Year Plans under Planning Commission of India starting from 1951 included some development programmes aimed at rural development and poverty alleviation. In this study the researcher has pointed out the limitations of the community development and empowerment plans implemented by the government and the non-government organisations with reference to Kondh community.

Keywords: Empowerment, Community, Development, Plans

INTRODUCTION

Since obtaining independence from the British in 1947, India has been trying to tackle problems of poverty and under development, on a war footing. India's share of the global GDP has come down from 24% to 3% during the two hundred years of British rule (Dutt, 1902). Lopsided colonial policies led to famines, which were felt hardest in rural India. An industrial revolution and subsequent import of British goods had greatly impacted Indian industry and village economy. The 'self-sustaining' Indian rural economy, where in most villages were having an economic eco-system, was broken'. India was largely left as an agriculture based commodity producer (Dutt, 1902). The Indian government under the leadership of Jawaharlal Nehru (1950), had decided to follow the centralized planning model of the then Soviet Union. National development plans were envisaged as five-year duration plans under the 'Planning Commission of India'. The first plan was started in the year 1951 and this model continued until the year 2015. The planning model was conceived by P.C. Mahalanobis and was known as the Mahalanobis Model. It envisaged a four-sector planning strategy with emphasis on heavy industries like Steel (A. Mitra, 1957).

India, on independence, had debated a Gandhian, bottom-up village as center based development plan, called as 'Kumarappa Plan' (Kumarappa, 1945). However, history tells us that the then Government of India and its leadership opted for centralized planning. This meant that even though India had gained independence largely on Gandhian leadership and thought (Gandhi, 1910), it was not followed in the economic development plans.

Rural Development Plans in India

There has been Five Year Plans under Planning Commission of India starting from 1951. Over the next 50 years, each plan period included some development programmes aimed at rural development and poverty alleviation. The following table gives an indicative list of such programmes.The model of centralized planning was finally aborted in the year 2015 and the central planning conversion was implemented as a national think tank. The focus of poverty alleviation had been built on the belief that there would be trickle down from economic growth and focus on specific political priorities. By 2015 it was finally concluded that the strategy largely did not work in the first 50 years of development (especially on rapid poverty alleviation), due to the following reasons:

a. The overall growth rate of the Indian economy itself was about 3% per annum in the first 40 years of independence (derided as 'Hindu rate of growth 'by noted Indian economist, Prof Raj Krishna).
b. The political priorities kept changing from 'infrastructure' development to focused individual or family level poverty alleviation.

While India avoided large-scale famines, and built reasonable industrial and educational infrastructure, poverty alleviation did not happen at a rapid rate (Gaiha, 2008; Ranganathan, 2012; Suresh, 2012; World Bank, 2011). There was an admission by the leaders that only 17% of the funds intended for poverty development reached the poor, as most development was executed 'for the poor' by the state apparatus with very little participation of the people in focus.

This understanding led to belief that India needed to refocus on village panchayats and give greater importance to the Gandhian model of village democracy. The 73rd and 74th amendments to the Indian constitution were finally passed in 1992, where 29 items of development administration were supposed to be directly transferred to village panchayats. Apart from the federal and state governments, the third tier, village panchayats became legitimate constitutional entities. In a way, the bottom up planning or development of villages and poverty alleviation has been mandated as all plans were to be passed in 'Gram Sabhas'.

Evaluation of the Developmental and Empowerment Plans

The researcher has more than 25 years of experience in working with Government and Non-Government Organisations for the development and empowerment of rural poor in India and has mostly worked with the Khond community, a local Adivasi or tribal community covering 50 villages. Khond community mostly resides in Southern and Western parts of Odisha. They were considered 'less developed' than the rest of the tribal communities.

The status of the centralized plans and programmes of the govt. already implemented had failed especially with the Adivasis or the Tribal community.
The following few examples illustrate the failures:

1. The State tried to promote dairy business as an income generating activity, only to realize that most of these communities treat milk as either puss or meant for calf and do not believe in touching it.
2. The State tried to promote tea plantation on a large tract of land that would have displaced over 12 villages. The plan was to employ the people as laborer in the tea garden. But the Adivasis were not used to industrial work culture and were not interested.
3. The State tried to promote gem and precious stone processing, as the area was rich in precious stones. But the Adivasis had no value for such stones and would not be interested to migrate for work.

4. A large horticultural tree plantation failed as the people uprooted all the trees overnight. Land meant for food crops was diverted to horticulture without their consent.
5. On occasion, such failed interventions also led to leaks and corruption. For example, equipment given for paddy processing or improved pottery was resold back to the same suppliers as the people did not know how to use it and there was no market for improved products. Many cases the suppliers simply bought back the equipment at throw away prices from people and re-circulated it to others.

Evaluation of Projects Implemented in the Field

The researcher himself worked in several projects as project lead. Most projects were planned with communities using Participatory Rural planning process (Robert Chambers, 1983). It involved meeting the communities frequently and staying with them. The process involved mapping local needs, local resources and then develop local solutions based on local capabilities. It is a practical adaptation of Freire's (1965) critical consciousness, empowerment framework. Further, the researcher has actively engaged in many such intervention including Women empowerment through self-help groups in large scale, Financial inclusion, Skill development for livelihoods creation, Education integrated with livelihood development skills.

The following observations have been made on the projects implemented at the ground level:

1. Even after so much of development experience and reading, most of the development intervention approaches continue to fail to understand the communities. We do not seem to know what works and what does not work. Even the experience of facilitating the participatory exercises leaves one dissatisfied that somehow the communities did not seem to own the outcomes.
2. Indian state still fails to understand these communities. Most programmes run on trial and error and it is difficult to predict the fate of an intervention beforehand.
3. This leads to a great deal of wastage and sometimes damage to the community too. The development interventions have promoted modern medicine, agriculture and education. In the process, the Adivasis traditional knowledge systems seem to be impacted. The modern systems also do not seem to deliver the results.

Case Studies to Understand Which Empowerment Approach Works & Which Does Not

Most participatory development approaches believe in community empowerment. Most empowerment theorists have emerged out of the seminal contribution of Paulo Freire (1965). The following examples highlight the need to revisit these concepts:

Case-1: Thaumal Rampur is in the Kalahandi district of Odisha, in the East of India inhabited by Khond community. While it has copious rainfall and hilly terrain, most of the people have problems of food supply. So, we were trying to introduce many crops. Pineapple was one such crop. However, while all agreed in a community meeting to grow pineapple, they would never end up taking the plants for growing. Upon enquiry, it was found that since most 'have never seen or tasted' pineapple, they were not sure. The problem was solved by introducing the people to pineapple and allowing them to taste it. It was a question of 'exposure' that led to action. So, does 'exposure' place limits on empowered action?

Case-2: The Khond community would take only one crop in their lands. In the case of a second crop, no one grew it even though there was food shortage and there was enough water for the crop. It was later found that since there is an open grazing problem, unless the whole community decided to grow a second crop, it would not work. So, do community level practices place limits on empowered action?

Case-3: In the case of 4000 odd self-help groups in the Gajapati district of Odisha, it was found that even after four years of sustained and programmed intervention, not even 10% of the groups developed the capability to reduce

their own poverty. The target was that at least 50% would be able to reduce their poverty. Was it due to inefficient programme capacity or were there other community level reasons?

Case-4: In the last ten years, skill development is used as a means of poverty reduction. Skill development, followed by migrant working, has moved many families out of poverty. But despite many such success stories, there has been little demonstration effect. People do not seem to be automatically motivated by the success of their peers. So, does that mean that exposure alone does not work?

Case-5: Sometimes even government regulations mandating empowerment do not produce desired results. For example, Indian government has mandated that 33% of the local elected representatives must be women. Seats are reserved for them. However, in many communities' women are unaccustomed to sitting with men and do not decide on public matters. In many places, it is found that even though women are elected, their husbands chair the meetings with the consent of wife.Often societal norms seem to play an enabling or disabling role. People tend not to do things or do things because of societal norms or rules. This is especially true when one looks at communities that have very layered labyrinth of 'lived experiences'. Sometimes habits, culture and beliefs also seem to determine the actions. For example, the researcher has come across cases where severe burns cases were considered as God's curse and 'waiting to die' and not allowed to go to hospitals. Communities used to pray to God seeking peaceful death. Cows are not milked because of social beliefs.

CONCLUSION

It is mostly trial and error to identify what works and what does not with regard to the developmental and empowerment programmes. One needs to dig deep to find reasons as to why a certain thing has happened or not happened.Such behavior is explained away quoting structural constraint, prolonged colonization or oppression (Freire, 1968). Some also argue that long term colonization leads to mental conditioning that is difficult to come out (Fannon, 1961). But continuation of such behavior even after such a long time after independence, even after people have tasted success and there is example in the vicinity makes one wonder as to whether there are other reasons too?

REFERENCES

1. Freire, Paulo (1961), Pedagogy of the Oppressed, Continuum international publishing group, London
2. Gandhi, M.K. (1910), Hind Swaraj or Indian Home Rule, published by Navajivan Publishing House, Ahmedabadad.
3. Parsons, Talcott (1964), 'Evolutionary universals in society', American Sociological Review, Vol 29, p.339
4. Kumarappa, J.C. (1945), Economy of Permanence
5. Mitra, A. (1957), 'A note on the Mahalanobis Model', March 16, 1957, The Economic weekly
6. Rappaport, J. (1984), 'In praise of paradox: a social policy of empowerment over prevention', American journal of community psychology,9, p1-25.
7. Gaiha, Raghav (2008), 'Poverty alleviation programmes in rural India: An assessment, pp2-38, Development and Change, Vol22, issue 1, 2008
8. Ranganathan (2012), 'Poverty Alleviation programmes in India-policy perspectives', International Journal of innovative research and development, October,2012
9. Suresh (2012), 'Poverty alleviation programmes in India and its consequences', Review of arts and humanities, Dec,2012
10. World Bank (2011), 'Social protection for a changing India', a report

Table 1: Plan Period-wise Rural Development Programmes:
(Note: Most plans are for five years. However, sometimes due to war, plans were curtailed for a few years).

Plan Period	Programmes	Key Focus
First plan (1952,53)	1. Community Development Programme 2. National Extension Service	Heavy industries like steel and establishing a government extension staff till the village level
Second Plan (1957-60)	1. Intensive Agriculture Development 2. Tribal Development Multi-Purpose Block level programme 3. Khadi and Village Industries Development 4. Village Housing	Agriculture productivity and rural industries and village housing
Third Plan (1962-66)	1. High Yielding Varieties programme 2. Rural Industries 3. Agriculture Development 4. Nutrition Programme	Start of 'green revolution'; a combination of provision of high yielding seeds, chemical fertilizer and extension support. A response to PL 480 US food grain support
Annual Plans (1967, 1968)	1. Farmers' training scheme 2. Rural Works 3. Tribal Block development 4. Women and Child programme 5. Well construction programme	Focused programmes on farmers, women and children. The approach was mostly sectoral development in nature
Fourth Plan (1970-74)	1. Drought Prone Areas programme 2. Small Farmer Development Agency 3. Rural Employment programme 4. Tribal Development programme 5. Minimum Needs programme 6. Command Area Development	Focus on large-scale welfare or social security schemes. Also on focus was on special area development needs
Fifth Plan (1975-79)	1. Food for Work 2. Integrated Rural Development 3. Training of Rural Youth for Self-Employment 4. Special Livestock Development 5. Desert Development	Focus on individual level poverty alleviation through training and livelihood linked programmes
Sixth Plan (1980-83)	1. National Rural Employment Programme 2. Prime Ministers 20-point new programme 3. Development of Women and Children in Rural areas 4. Rural Landless Employment Guarantee	Large-scale rural wage employment programmes; Focus on women and children and landless people
Seventh Plan (1985-86)	1. Rural Energy 2. Livestock Breeding programme	Focus on specific areas; debate on utility of centralized programmes starts

Eighth Plan (1989-93)	1. Rozgar Yojana 2. Prime Minister Rojgar Yojna 3. Employment Assurance Programme	Focus on organized wage employment and individual livelihoods promotion; The attempt to start empowerment based bottom-up planning gets a boost with the 73/74 constitutional amendments;
Ninth Plan (1996-02)	1. Basic Minimum Services 2. Swarnajayanti Swarojgar Yojana 3. Jawahar Gram Samrudhi Yojana 4. Swajaldhara	Focus on some centralized programmes and some money given as block grants for bottom-up planning
(2014-17)	1. Employment Guarantee programme 2. JAM (Jandhan, Adhar, Mobile) 3. Block grants	Present focus on financial inclusion; a few centralized social safety schemes coupled with panchayat level bottom-up development plans.

Source: Five-Year Planning Documents of Government of India, Planning Commission.

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RESEARCH ARTICLE

Necessity of Implementing Technical Writing in Engineering Curriculum: Challenges vs. Benefits

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ABSTRACT

In the time of assistive technology tools and auto-correct apps, students within the engineering and technology fields face a few difficulties in moving to writing activities of extensive length and intricacy, regardless of whether through restricted involvement in written projects or could likewise be an individual lack of engagement in the act of writing. Engineers regularly accept technical writing to be profoundly point by point documentation including diverse undertakings beginning from writing assignments, contextual investigations, specialized reports, research facility reports, assessment inquiries through writing articles in diaries to definite year thesis. This thought over weights the researchers to adapt up to the educational program which at that point prompts dissatisfaction and lackluster. There are complaints from managers about the poor writing abilities among engineering graduates. By and large, there are three viewpoints that students who study engineering face challenges when writing scholarly articles in for example substance, structure and language. Characteristically to fortify the standard of instructive composition among engineers, these angles must be taken into consideration. On the opposite, numerous association have now moved their have practical experience in improving the correspondence and expert skills by overcoming any issues between diagnostic reasoning and logical correspondence of the engineering students. Professional communication skills and technical expertise are equally important in industry. In any case, customary, humanities-based writing courses are frequently the main proper writing readiness accommodated designing students. But, while the humanities offer courses that order interpretive, pugnacious, and logical composition, engineering students regularly ignore comparative thinking styles among designing and hence the humanities on account of the obvious distinction in the content taught. This paper discusses what are the difficulties and the manner in which they will become benefits and recognize procedures for architects to acknowledge extraordinary specialized writing. This paper additionally centers around the need of usage of a Technical Writing and Communication course that looks to upgrade regions of industrious open test for engineering students populace.

Keywords: Technical writing, communication, collaboration, strategies

INTRODUCTION

One of the key difficulties students in engineering and technology face is capability in technical writing. Generally, graduate instruction is intended to prepare students for instructive examination at the doctoral level, or for cutting edge positions in their order or for engineering up themselves in whichever profession they're in. It's abnormal to search out a program which doesn't require competent written and discourse skills as an objective or learning result for the graduate of that program. In any case, students go to the graduate level with varying degrees of skill in their capacity to introduce themselves through written language. Professional engineers are required to be ready to communicate effectively, including in written formats like technical reports (Engineering Council, 2014). Colleges intend to sort out undergraduates for the professional condition; in any case, numerous new budding graduates despite everything come up short on the degree of writing skills expected by their bosses (Moore and Morton, 2017), and 71% of overviewed designing managers have confronted issues since applicants have great specialized information yet need working environment abilities (Institution of Engineering and Technology, 2017).

Background of Study

The Engineering divisions at various specialized Universities of Odisha do not resolve to empower self-guideline in first and second year engineering students by urging them to ponder their composed work. Explicit teaching of writing skills isn't given and it anticipates that students should pick them up as they complete the rest of the educational program. By third and fourth year, undergraduate engineers are required to present a written record about their individual (third year) and group (fourth year) projects. These activities represent 33% of the year point every year. In first and second year, students follow a few compulsory unit covering core engineering topics. Evaluation for each unit commonly contains 75% test and 25% laboratory activities every year. A group contains up to hundred to hundred and fifty students, and laboratory sessions are delivered to smaller groups of thirty students at a time. There are a decent scope of appraisals utilized for laboratory work: a few units grant credit just for joining in; most require some grammar assignments or reading comprehension to be completed; few assignments on listening skills and a minority require a brief, report to be submitted. This assortment is not ideal for showing technical writings for a few reasons. To begin with, the deficiency of consistent expectations (even within the few labs that need submission of a written report) can confuse students. Second, there are just a predetermined number of chances to work on writing longer records, constraining the probability of being able to improve performance.

Third, it's not in every case clear how input from one report has pertinence to future assessments. These issues conflict with the recommendations made by Nicol and Macfarlane-Dick (2006) for helping students to turn out to be increasingly self-controlled behaviour. Instructors frequently communicated their mistake about the standard of instructive writing among students. Lectures consistently griped that they think that it’s hard to realize the researchers writing what more if the writing is finished not in their language and furthermore the writing included specialized phrasings for example engineering wordings. When they look at the magnificent scholastic compositions and consequently the ones that the researchers composed, they feel that the hole is wide. Anyway they have to comprehend that students need time to acclimate themselves which isn't sufficient to ace the specialized writing abilities in just eighteen months. It is genuine that occasionally students aren't focused on their work however the elements that cause such shortcomings must be inspected and rewarded appropriately.

One among the clarifications is on the grounds that students don't have a lot of introduction to scholastic composition and since speakers showing designing concentrated more on the substance perspective rather than the occasion of technical writings in students. There’s an observation that if instructors distribute some of their opportunity to show technical writings, this may end in the decrease of designation in center substance educating and learning. By the by creating scholastic perusing and technical writings at the same time, this may in a roundabout way reinforce students' perception of center substance (Wheeler and McDonald, 2000).On the other

hand students griped that the speakers expect an over the top measure of from them when really they are attempting to acclimate themselves with the instructional exercise condition. They felt that the change from school to the college might be a tremendous weight upon them. The researchers felt that the assignment of understanding the designing subjects itself might be a gigantic undertaking to manage. Consequently a considerable lot of them felt that the need of specialized writing adds to the current weight.

Issues and Challenges

Before the design and usage of the specialized composition and correspondence course for the students, the educational plans were bolstered by writing concentrated courses instructed in the humanities, which likewise add to an understudy's general training prerequisites. The writing courses were created more than forty years back as a "one size fits all" response to an outsized general education pre-requisite of the engineers graduating every year. With the extension of engineering students inside the previous decade, built up the specialized composition and correspondence course to fulfill the interest of designing staff and industry accomplices. While humanities-based writing courses despite everything be remembered for designing understudy advancement, these writing concentrated courses commonly are taken inside the first or second year, leaving engineering students without basic composition and informative course bolsters as they move past their sophomore year. Fundamentally, the execution of sending in designing training remains a challenge for two reasons. To begin with, designing instructors still can't seem to prevail in an accord about how writing ought to be educated and evaluated. Goldsmith and Willey note that while there's wide understanding in regards to desires, there remains contradiction among engineering instructors on the job of writing inside the educational plan, likewise as who will educate it.

Second, while wide includes expanded presentation to the humanities might be a typical subject in engineering curricular plan conversations, for all intents and purposes, it's hard to discover how this is regularly to be actualized without only adding one more year to the predominant , unbending course load necessities. Another commitment to the matter of poor writing abilities emerges from students not having a straightforward thought of what 'great' writing appears. Levels of self-guideline decide how well an individual can plan, screen and self-assess progress towards an objective, and better levels end in increasingly inspired, better-performing students (Bandura, 1991; Pintrich and de Groot, 1990;Zimmerman, 1986). On the off chance that an understudy cannot envision the objective, it is difficult to shape positive advancement towards it, so an understudy who cannot picture 'great' writing won't be prepared to deliver it. Great criticisms are regularly a valuable thing to create self-guideline in students, by helping them to find out how their exhibition analyzes to 'great' execution (Nicol andMacfarlane-Dick, 2006). On the other hand, results concentrate in subjective and learning science show that composition, when utilized in explicit ways, empowers students associate thoughts, look at information holes, and empowers LTM recovery.

All things considered, designing teachers' endeavors to utilize these methods of writing are blended. Utilizing supposed write-to-learn techniques in situ of writing as a kind of appraisal, engineering instructors formulated a self-intelligent writing brief that was offered iteratively to a class, and expected students to consider and assess their critical thinking approach. Notwithstanding, this course change yielded no connection with improved understudy execution on content-based tests. Writers hypothesize that execution are the guilty party, taking note of that their writing brief didn't expect students to join earlier information with new information. Psychological and learning science discoveries show that write-to-learn endeavors are compelling when two measures are met: student self-reflection and accordingly the capacity to effectively interface old and new knowledge. While Goldsmith and Willey note in another investigation note that if reasonable writing rehearses were to be effectively brought into designing educational programs, they may got the opportunity to introduce writing as a bonafide practice that architects do every day, and one that partners, builds in industry, and designing scholastics must do successfully. This shows the quandary that incorporating writing into existing designing educational programs keeps on being a challenge. The challenge is worth addressing— implementing a technical writing and communication course can provide two benefits: (i) tangible exposure to engineering writing conventions, and (ii) support for learning.

LITERATURE REVIEW

Past literary works have recognized that specialized writing are frequently characterized as a correspondence movement in managing and conveying specialized data and subjects like in technology, engineering, science and different fields with explicit wordings at specific working environments through composition (Finklestein, 2007; Indra Devi, Husin and Subatira, 2010; Laplante, 2012; Manivannan,2005; Pfeiffer and Adkins, 2010; Van Endam, 2005). This shows specialized writing is a pivotal aptitude to practically any calling including engineers, researcher, planners, doctors, lab experts then forward. Actually, work businesses requested likely representatives with sound specialized relational abilities including specialized composition (Kassim and Ali, 2010; Rhoulac & Crenchaw, 2006). Representatives in industry invested their energy generally in specialized composition, for example, working time from various occupation works in ventures is spent nearly on writing at the working environment like specialized composition (Mohd Raus, 2005; Nordin, 2013). By having specialized writing competency, one could pass on essential data obviously and precisely to concentrate on crowd with explicit reason (Laplante, 2012; Van Endam, 2005).The English language courses offered inside the designing projects expects to sort out students with required skills in scholastics and in specialized setting with the point of setting up the researchers for working in businesses.

In any case, it's discovered that specialized writing in English isn't completely executed and in this manner the appraisal of composed assignment doesn't contribute much inside the checking plan of English for correspondence course (Department of Polytechnic Education, 2011). Along these lines, students probably won't consider written to be in English as significant as different abilities. This may make a negative discernment towards writing in English. As expressed by Warnock and Kahn (2007), many engineering students consider writing to be random to their future vocation objectives. The present Communicative English courses at Engineering schools are educated over all orders whereby students of different fields like engineering, polytechnic, management, diploma , et al. take a proportionate English course. Along these lines, the schedule of current English courses probably won't be prepared to totally give the students' specific language needs with respect to example specialized writing course for engineering students (Sanmugam, 2013). An ongoing report by Lam and Chong (2013) have researched polytechnic students' recognitions on their learning encounters during their Communicative English course and uncovered that very a large portion of the researchers concurred that English language educational plan didn't assist them with enhancing their English.

While, an examination led by Md. Yasin et al. (2010) on English expertise inadequacies of polytechnic students, found that understanding specialized archives, utilizing right sentence structure, jargon and punctuation, writing test/examination report and addressing for explanation are among the significant skills that specialized students needed of. Steady with Mustapha et al. (2008), on an examination which decided preparation among students on K-economy and globalization featured about consolidating correspondence and exploration skills in specialized educational plan. Henceforth, information recorded as a hard copy a specialized logical exploration which can improve composed language abilities is in think to flexibly a skillful laborer. On the contrary hand, these are the gifts that students ought to procure additionally in light of the fact that the skills required by the enterprises (Md Yasin et al., 2010). In any case, 31.5% of jobless alumni in Malaysia were among moves on from polytechnic and ailing in composed language skills was one among the primary explanation that caused this issue (Esa, Selamat, Padli and Jamaluludin, 2014). In different investigations prior, gratitude to need relational abilities for both spoken and written in English, various number of the alumni from Malaysian polytechnics are jobless (Md. Yasin et al.,2010).

This may give negative think about the standard of polytechnic graduate. As expressed by Idrus (2008), the absence of researchers to gracefully great nature of writing, may reflect to the standard of the alumni's students of the association that they're have a place with. Thinking about the above issues of polytechnic situation, this examination attempts to fill the hole of specialized writing competency needs among engineering students at Malaysian polytechnic. Along these lines, this examination plans to investigate the specialized writing competency needs of the designing students at Malaysian polytechnic on the possibility of students' points of view. In particular, the targets of

this investigation are to work out the engineering students' see on their specialized writing competency as far as information, abilities and mentalities towards specialized writing in English and to explore the understudy's apparent on specialized writing competency needs. Lager and McMurrey (2009) propose that the matter of poor writing abilities emerges somewhat on the grounds that students who pick designing wish to represent considerable authority in scientific and viable work instead of composed work. This intrinsic inclination adds to a shortage of enthusiasm for creating writing abilities. Students can likewise underestimate the significance of technical writings (Lievens, 2012; Nguyen, 1998), which could additionally decrease inspiration to discover these abilities (Ramsden and Entwistle, 1981). Nonetheless, different investigations have demonstrated that students do perceive the significance of relational abilities in their future professions, yet less significantly than specialized skills . Direito et al. (2012) additionally found that students report an 'expertise hole' for a few delicate skills, including composed language, whereby they rate skills as significant, however don't accept they need a legitimate capacity in those skills. This absence of trust in capacity can cause students maintaining a strategic distance from the errand, so not having the possibility to rehearse and improve (Bandura, 1982).

Findings

One of the fundamental shortcomings is that the failure to discover the effortlessness in multifaceted nature. Poor capability of English language, poor sentence skills, core content, structure of writing, scholarly writing shows, examination of writing points; capacity to direct research and apply information across various setting (Pineteh, 2014). Such shortcomings are regularly seen among students who study subjects like engineering during which a few students respect scholastic writing not significant contrasted with the center substance. Naturally, writing is overlooked in light of the fact that it is thought not valuable for their future career. Investigations have demonstrated that the clarifications for the poor writing capability are: (1) issues related with the educators themselves for example poor disposition, deficient instructive abilities and information, (2) specialized viewpoints required in explicit skills, (3) the educating and learning forms used the inaccurate showing methodologies and (4) unsatisfactory evaluation. Typically, the issue is said to either the educator or the instructing procedure. Some of the issues are somewhat connected with the instructor likewise because of the educating and learning forms and a couple additionally as a result of the researchers themselves (Kamaruddin and Abdullah, 2015).

Benefits of Learning Technical writing

Skill in specialized writing in English may be another incentive to any future workers when looking for work since English has become an essential and worldwide mechanism of correspondence broadly. Truth be told, by having great specialized technical writings will permit students to be able in relational abilities and should give them a credit when applying work (Laplante, 2010; Tebeaux, 1983). An examination on engineering up a substitution abilities standard to flexibly information specialist in Malaysia had distinguished that laborers are required to reinforce their competency which encourages them to hold out their activity well (Ismail, Mustapha, Spottl, and Md Yunos, 2013). Since English might be a worldwide language, laborers got the chance to be skilled with the planet language to widen their insight. Moreover, managers look for up-and-comers who have brilliant scholastic execution as well as have great relational abilities in both spoken and composed English (Ngah, Mohd Radzuan, Fauzi, and Zainal Abidin, 2011; Nordin, 2013; Raftopoulas, Coetzee, and Visser, 2009; Raybould and Sheedy, 2005).

Along these lines, the keys to progress inside the engineering calling is that the capacity to talk in both spoken and composed English (Bonk, Imhoff, and Cheng, 2002). Furthermore, writing abilities in English was seen as significantly significant as talking and listening skills for section level work (Zubairi, Sarudin, Nordin, and Tunku Ahmad, 2011). Students ought to be shown specialized composition at an early age to build up the motivation of specialized writing in English (Herzogs and Hinds, 2015). Thus, students who can't record well in English are at a major block. Consequently, specialized writing competency in English has become an a sound representative for have to any new alumni in work enterprises (Kassim and Ali, 2010;). The examination has demonstrated that the Technical Writing course might be a crucial segment inside the preparation of a designer to ensure that when the researchers graduate, they are familiar journalists who can meet the pressure of writing inside the engineering

calling. Specialized writing ought to be carefully presented inside the Engineering educational program and given satisfactory chance to manage all the points involved inside the course and given sufficient opportunity to rehearse the ability by the researchers. Coordinated effort between speakers of educators encouraging English and instructors of engineering is huge all together that the past are frequently aware of the students' writing issues that the last experience inside the students' composed work. That way, the engineering speakers will be assuaged of the weight of tending to language issues and just think about the substance, while the writing issues are tended to by specialists.

CONCLUSION

All in all, engineers in training got the opportunity to ace the aptitude of writing generally and technical writing particularly. The Technical Writing course is accordingly an extremely significant part in designing instruction. it's helpful during and in the wake of preparing on the grounds that it adds to an engineer's prosperity at the college and inside the business life . During preparing, a engineering understudy must compose plainly the undertakings given by teachers. Absence of clearness during an understudy's work may end in bad grades, and thus less odds of accomplishment. So also, an architect who could likewise be a familiar author might be perceived by the board and should increase quickened advancement than a specialist who is a little capable in writing. Hence, the engineering educational program planners ought to understand its significance of getting such a course for the designing alumni which could order creating top quality architects and help in adding to the expansion of their nations 'economies through science, engineering and technology and therefore contend all around.

REFERENCES

1. A. S. Horning, "Defining Literacy and Illiteracy", The Reading Matrix, vol. 7, no. 1, p.73, April, 2007.
2. Allen, J. (1990). The case against defining technical writing. Journal of Business and Technical Communication, 4(2), 68–77. doi:10.1177/105065199000400204 [Crossref], [Google Scholar]
3. Bandura, A. (1982). Self-efficacy mechanism in human agency. American Psychologist, 37(2), 122–147. doi:10.1037/0003-066X.37.2.122 [Crossref], [Web of Science ®], [Google Scholar]
4. Bandura, A. (1991). Social cognitive theory of self-regulation. Organizational Behavior and Human Decision Processes, 50(2), 248–287. doi:10.1016/0749-5978(91)90022-L [Crossref], [Web of Science ®], [Google Scholar]
5. Beer, D., & McMurrey, D. (2009). A guide to writing as an engineer. USA: John Wiley & Sons, Inc. [Google Scholar]
6. Boekaerts, M. (1997). Self-regulated learning: A new concept embraced by researchers, policy makers, educators, teachers, and students. Learning and Instruction, 7(2), 161–186. doi:10.1016/S0959-4752(96)00015-1 [Crossref], [Web of Science ®], [Google Scholar]
7. Carter, M.J., & Harper, H. (2013). Student writing: Strategies to reverse ongoing decline. Academic Questions, 26(3), 285–295. doi:10.1007/s12129-013-9377-0 [Crossref], [Google Scholar]
8. Direito, I., Pereira, A., & Duarte, A.M. (2012). Engineering undergraduates' perceptions of soft skills: Relations with self-efficacy and learning styles. Procedia - Social and Behavioral Sciences, 55, 843–851. doi:10.1016/j.sbspro.2012.09.571 [Crossref], [Google Scholar]
9. Emig, J. (1977). Writing as a mode of learning. College Composition and Communication, 28(2), 122–128. doi:10.2307/356095 [Crossref], [Google Scholar]
10. Engineering Council. (2014). UK-SPEC UK standard for professional engineering competence(3rd).
11. Fulwiler, T. (1984). How well does writing across the curriculum work? College English, 46(2), 113–125. doi:10.2307/376857 [Crossref], [Web of Science ®], [Google Scholar]
12. Gibbs, G., & Simpson, C. (2005). Conditions under which assessment supports student's learning. Learning and Teaching in Higher Education, 1, 3–31. [Google Scholar]
13. Grossberg, K.M. (1978). ERIC/RCS report: The truth about technical writing.The English Journal, 67(4), 100–104. doi:10.2307/815643 [Crossref], [Google Scholar]

14. Institution of Engineering and Technology. (2017). Skills & demand in industry 2017 survey. UK: IET. [Google Scholar]
15. Itani, M., & Srour, I. (2016). Engineering student's perceptions of soft skills, industry expectations, and career aspirations. Journal of Professional Issues in Engineering Educations and Practice, 142(1), 04015005-1–04015005-12. [Web of Science ®], [Google Scholar]
16. Kinneavy, J.L. (1983). Writing across the curriculum. Profession, 13–20. [Google Scholar]
17. Lievens, J. (2012). Debunking the 'nerd' myth: Doing action research with first-year engineering students in the academic writing class. Journal of Academic Writing, 2(1), 74–84. doi:10.18552/joaw.v2i1 [Crossref], [Google Scholar]
18. Martin, R., Maytham, B., Case, J., & Fraser, D. (2005). Engineering graduates' perceptions of how well they were prepared for work in industry. European Journal of Engineering Education, 30(2), 167–180. doi:10.1080/03043790500087571 [Taylor & Francis Online], [Google Scholar]
19. McPherson, G., & Zimmerman, B.J. (2011). Self-regulation of musical learning:A social cognitive perspective on developing performance skills. In R. Colwell& P.R. Webster (Eds.), MENC handbook of research on music learning (pp. 130–175). Oxford, UK: Oxford University Press. [Crossref], [Google Scholar]
20. Melin Emilsson, U., & Lilje, B. (2008). Training social competence in engineering education: Necessary, possible or not even desirable? An explorative study from a surveying education programme. European Journal of Engineering Education, 33(3), 259–269. doi:10.1080/03043790802088376 [Taylor & Francis Online], [Google Scholar]
21. Moore, T., & Morton, J. (2017). The myth of job readiness? Written communication,employability, and the 'skills gap' in higher education. Studies in Higher Education, 42(3), 591–609. doi:10.1080/03075079.2015.1067602 [Taylor & Francis Online], [Web of Science ®], [Google Scholar]
22. National Center for Academic Transformation. (2006, April). The learning marketspace. NCAT Newsletter. Retrieved from http://www.thencat.org/Newsletters/Apr06.htm [Google Scholar]
23. Nguyen, D.Q. (1998). The essential skills and attributes of an engineer: A comparative study of academics, industry personnel and engineering students. Global Journal of Engineering Education, 2(1), 65–75.[Google Scholar]
24. Nicol, D.J. (2010). From monologue to dialogue: Improving written feedback processes in mass higher education. Assessment & Evaluation in Higher Education, 35(5), 501–517. doi:10.1080/02602931003786559 [Taylor & Francis Online], [Web of Science ®], [Google Scholar]
25. Nicol, D.J., & Macfarlane-Dick, D. (2006). Formative assessment and self-regulated learning: A model and seven principles of good feedback practice. Studies in Higher Education, 31(2), 199–218. doi:10.1080/03075070600572090 [Taylor & Francis Online], [Web of Science ®], [Google Scholar]
26. Pintrich, P.R., & de Groot, E.V. (1990). Motivational and self-regulated learning components of classroom academic performance. Journal of Educational Psychology, 82(1), 33–40. doi:10.1037/0022-0663.82.1.33 [Crossref], [Web of Science ®], [Google Scholar]
27. Ramsden, P., & Entwistle, N.J. (1981). Effects of academic departments on students' approaches to studying. British Journal of Educational Psychology, 51(3), 368–383. doi:10.1111/bjep.1981.51.issue-3 [Crossref], [Google Scholar]
28. Robinson, C.M., & Blair, G.M. (1995). Writing skills training for engineering students in large classes. Higher Education, 30(1), 99–114. doi:10.1007/BF01384055 [Crossref],[Web of Science ®], [Google Scholar]
29. Selwyn, R., Renaud-Assemat, I., Lazar, I., & Ross, J. (2018, July). Improving student writing skills using a scaffolded approach. In Proceedings of the 7th International Symposium for Engineering Education. University College London, London, UK. [Google Scholar]
30. Twigg, C.A. (2015). Improving learning and reducing costs: Fifteen years of course description.Change: the Magazine of Higher Learning, 47(6), 6–13. [Taylor & Francis Online], [Google Scholar]

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RESEARCH ARTICLE

Who Adopts What, Where, When, Why and How?

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ABSTRACT

Change is the goal of teaching English (Boraie, 2013). The new trends, methodologies and pedagogies today aim at internalising what is learnt rather than just knowing and acquiring. The emergence of the modern trends due to Westernization in Literature has impacted Indian education system. It has taken the initiative and introduced innovative and interactive study like smart classrooms, online chat sessions and interactive language labs. This is an era of innovation. The whole generation has changed. The new generation is addicted to computer, social networks. This affects their styles of learning and how they react to the teaching of a teacher. There is a need to exploit the modern methods which respond to the needs and interests of these learners. Since students come from different cultural and linguistic backgrounds with different learning styles and capabilities, it is essential that a spectrum of teaching methods and materials must be explored and traversed. The innovative ingenious teacher is capable of drawing out information from texts, videos, audio sources of information for teaching purposes. This paper seeks to explore and motivate the many ways of making the out-of-the-box teaching a possibility and a reality, bringing in innovation right into the classroom.

Keywords: Innovation, Learning Practices, Trends, English language

INTRODUCTION

Even though English is an adopted official language in India, the learners face difficulties, one of the main reasons being that every Indian, belonging to any state, has his or her own mother tongue. The learners feel compelled to learn English as a second language. Change is the goal of Teaching English (Boraie, 2013). The new trends, methodologies and pedagogies today aim at internalising what is learnt rather than just knowing and acquiring. The emergence of the modern trends due to Westernisation in literature has impacted Indian education system. It has taken the initiative and introduced innovative and interactive study like smart classrooms, online chat sessions, interactive language labs. This is an era of innovation. The whole generation has changed. The new generation is

hooked to social networks. This affects their styles of learning and how they react to the teaching of a teacher. There is a need to exploit the modern methods which respond to the needs and interests of these learners. Since students come from different cultural and linguistic backgrounds with different learning styles and capabilities, it is essential that a spectrum of teaching methods and materials must be explored and traversed. The innovative ingenious teacher is capable of drawing out information from texts, videos, audio sources of information for teaching purposes. This paper seeks to explore and motivate the many ways of making the out-of-the-box teaching a possibility and a reality, bringing in innovation right into the classroom. Innovations are imperative for bringing an improvement in the motivation and effectiveness of teachers. As stated in the Twelfth Five Year Plan, education requires revolutions in the fields of methods of assessment of students learning, enhanced training of teachers, pioneering and creative pedagogies in the classrooms especially that which encourages technology in classroom.

Problem Statement

An estimated 1.5 billion English language learners are there world-wide (Beare, 2018). From 1800s to the present day, so much has changed which can be exciting or terrifying but the one thing which has not changed is the classrooms, which shows that there is a need of a teacher inspite of the fact that education is becoming highly technical. The education system in India is following an outdated pedagogy. The teacher-centred pedagogy and mode of teaching has been dominant for more than a hundred years. In this exam-oriented system of instruction, the teacher as a narrator infuses knowledge into the students through a parrot-like imitative process. Teachers find it challenging to hold on to the interest and the attention of the student throughout the teaching period. As soon as the class begins, the attention of the students starts wavering, and by the end of the class there is rampant boredom. Teachers knowingly or unknowingly discourage and ignore the participation of the students. When given a chance the minority extroverts dominate the class and thus deprive the majority introverted students from participation. Lack of motivation for learning induces lack of interest in the students, thus declining the performance of the students. The major challenges are faced by students coming from rural and underdeveloped areas, tribal background, economically backward society and uneducated families.

There should be a smooth and gradual transition from the usage of mother tongue to the second language i.e. English. This would help the children to express themselves. The transition requires that the students be provided with suitable vocabulary or structure as well as motivating students to use English for communication. This can be achieved by providing a secure and stimulating natural environment for language learning. The use of English language gives new openings and opportunities at the international front. On the one hand, we have innumerable people who are keen to learn, read, write and speak English but variety of these learners and their qualities, location and circumstances have made English language and its teaching a hard nut to crack. Use of innovative practices seems to be the only rescue to the new horizon of English language teaching (ELT). The field and perspective of ELT is really multi-facet but we need to step forward very cautiously to make English likeable and enjoyable to everyone.

Inspite of the lacuna in the present traditional way of education, a number of students and teachers still have a preference for it. The teachers are not sure about the feasibility of implementation and effectiveness of innovation, which is why the teacher-centred pedagogy is still preferred. This is because the teachers lack the open-mindedness for the innovative trends as they are not methodology savvy. They are hesitant in applying innovative approaches in their classes. Teachers are called upon to give away the outdated roles and act more as guides and mentors, exploring the new media themselves as learners, and thus acting as role models for their learners. Innovation will be essential to bring about qualitative changes in education, as opposed to the quantitative expansion seen so far. These changes are needed to enhance efficiency and improve the quality and equity of learning opportunities. Although education is not averse to changes, with improvements already taking place in classrooms, it has not managed to harness technology to raise productivity, improve efficiency, increase quality and foster equity in the way other public sectors have. At the same time education can also encourage innovation in society at large by developing the right skills to nurture it. These skills, including critical thinking, creativity and imagination, can be cultivated through appropriate teaching, and practices such as entrepreneurship education. Smart innovation strategies

developed by the Government for education with the right policy mix, will give meaning and purpose to innovation, including creating an innovation-friendly culture. Practitioners who are engaged in any innovations related to language education, need to have a framework consisting of the following composite questions, who adopts what, who adopts where, who adopts when, who adopts why and how, with responses to each individual component of the question, thus defining the basic issues that are of interest to the practitioners.

Objectives

- To overcome the challenges by integrating innovative practices in the classroom (seek to inform, to motivate and to explore the many possibilities of making out-of-the-box teaching a reality)
- To design a guideline to overcome the challenges of learning

Defining Who

Teachers play a vital role in an attempt to promote innovations when designing syllabus. There would be other people also like officials of the Education department of the government, deans, department heads, heads of the institutions, who would be playing a part in this process of promoting innovation, by implementing the innovations. Students as patrons, curriculum designers as dealers and the expat curriculum expert play their roles in this process of adopting and adapting innovation. Teachers may become adopters or sometimes they may become change agents. However, all the above, except the change agents, may also oppose an innovation and innovative practices. Thus, it can be concluded that a wide variety of people in the society are involved in any type of innovative practices in English Language Teaching.Adoption may also be hypothesised in terms of levels of execution, a measure which specifies the profundity to which any changes have occurred. Research has shown that it is difficult to promote innovation at a fundamental level. It should be remembered that innovations need to stand the test of time, for generally seventy five percent of the innovations fail as they are neither adopted in a proper way nor are they able to sustain the change.

Defining What

Innovation in terms of materials, the various teaching approaches and values, refers to qualitative changes in education. It is imperative in terms of evaluation of new methodology or assessment.

Defining Where

The question of where an innovation is applied is perceived in socio-cultural terms. Experts who wish to introduce innovative syllabi into an educational system must recognize the potential impact (whether positive or negative) of various socio-cultural constraints on their activities. It is necessary to identify the various factors related to culture, ideology, history, politics, economy, administration, institution, society and language, as they affect the implementation of any innovative project. Some effort has been made to establish the relative importance of these factors. For example, Kennedy (1988) envisions classroom innovation as being constrained by multiple systems, in which, as shown in Figure 1, cultural values are the most powerful shapers of behaviour, followed by political conventions, administrative practices, and others. The constraints shown in the Figure 1 cannot be accounted for in a discrete or a linear fashion. Experience suggests that all the subsystems, which are interrelated, have an impact on all the aspects of how innovatively a syllabus is designed, how well it can be implemented and how it would be evaluated.

Defining Why

There are many varied reasons why innovations are adopted or rejected. It is noted that all individuals do not adopt a change in the same way as it depends upon the different psyche of the people which influences their behaviour towards adopting change. For example, it is interesting to note that those who travel widely are well-educated because they adopt to the change early. These people are open to new innovative ideas being broad-minded and they have a vast exposure to mass media. They associate with others extensively and are extremely resilient as they know

how to deal with the uncertainties. On the other hand, the dawdlers are seen to have exactly the opposite characteristics whereas the people who are neither very open to nor are they opposed to new ideas, display intermediary traits.The adoption or inhibition of innovations depends on their characteristics and traits. The most well-known attributes derived from some 1500 empirical and/or theoretical studies have been used here as proposed by Rogers (1983). These characteristics or attributes comprise the following:

- the advantage gained by a possible adopter planning to adopt an innovation
- the compatibility of the innovation with previous practice
- the complexity and complication of the innovation
- the ability for trials of the innovation
- and the observability of the innovation

Defining How

There are different theories existing which seek to account for how change and innovation occurs. People can be persuaded to adopt an innovation. This requires planning, developing, testing, production, distributing to potential users. Though the initial cost of development may be high but the long-term benefits with respect to efficiency and the high quality of the innovation is worth mentioning. Today, in this global world, there is a sincere honesty towards using modern ways in teaching English on a continuous basis. This demands for teaching, learning, thinking and behaving. In the present ever changing world, it is required that an environment is created to ignite the way learning is done by giving a creative atmosphere. The purpose of the research is to find out different innovative ways that are going to inspire learners and teachers to transact the language in the most appropriate manner, so as to benefit the learner lifelong. Thus, a multidisciplinary framework, on innovation in language planning is to be developed based on the review of the problems that define innovation in the specific context of English language teaching.

A system which is audacious in inspiring experimentation and innovation, involves itself in regular reviewing of the learning outcomes would always be progressive. The education of the teacher should not be excused in this case. Pedagogical knowledge has to constantly undergo adaptation to meet the needs of diverse contexts through critical reflection by the teacher on his/her practices. The teacher needs to develop an open mind to encompass the differences in the cultural aspects and varied learning and teaching approaches to be more humanistic in his/her approach to traversing the knowledge to the students in the class in a more innovative manner.

Howard Gardner (2008) makes an interesting observation in his book Five Minds. He elucidates that innovation and creative thinking is at the centre and at the heart of any schooling. He describes the attributes of a well-organised mind and a creative mind which in turn lead to a creating mind. He further articulates that it is necessary to learn thoroughly at least one discipline and learn to hone and understand the skill, so as to be successful in the future. The synthesizers should be able to objectively understand and evaluate the information obtained from disparate sources and put it in a way that works both for themselves and for the others. The creating mind puts forward new ideas using discipline and synthesis as the base. The not so familiar questions attribute to a fresh way of thinking which further accentuates innovation.

Some Innovative Approaches to Language Teaching

Today there are new ways of supporting teachers and learners. There is a need to upgrade education skills to education 3.0 as education should be transacted beyond classrooms. English is an access to the 21st century skills. Today's teaching and learning of English is based on tech-in-hands education. A few ideas towards ELT which are innovative:

- Active and student centred apps
- Active learning through E-Book
- Create an E-Book for publishing to increase student engagement
- Modern adaptation of a traditional children's story
- Use collaboration in writing as a means for students to learn from their peers
- Share and comment on peers' work in a common digital platform, in order to create accountability and to provide a real life experience
- Video clippings
- Role playing
- Google space for students
- Students develop the curriculum and content
- Students in different countries connect and communicate
- Skyping
- Flipped Classrooms
- Gaming and mindcrafting
- Describe small video clippings creatively

The 'convent education' and this type of education which has remained the exclusive privilege of the rich, is a general craze in the society. Again, the standard of English teaching in Indian schools (with the exception of a few elite schools) has fallen dramatically, chiefly because infrastructure has not been able to keep up with the exploding number of students. But the role and importance of English in the Indian society continues to rise unrestricted. Vernacular and mother tongue education continue to be neglected. Thus, while Hindi remains the 'official' language, English continues to rule the roost. Problems caused by this phenomenon are indeed difficult to resolve. A lot of responsibility is left for English teachers to make their classes interesting and fruitful earning. Against this background, we need to find a solution to these challenges. If the solutions are sought for, it is realized that they are not in the hands of the teachers. These challenges can be turned opportunities and teachers can become resourceful. Open ended activities certainly can improve the quality of ELT class.

Activities which are open-ended are recommended to students so that they can work on their own rules with the help of their learning styles, find out their interests and produce work which is most appropriate to their capabilities. Innovation comes when the teacher does not expect the same type of work from everyone, though he/she gives the same activity and same set of instructions. This reflects the responsiveness of the students in terms of their interests and capabilities. The independent and challenging situation may be maintained in the class through powerful instructional strategies which help in differentiating learning experiences. In this way their learning is aligned with the learning experience.

CONCLUSION

Putting the idea in a nutshell, the role of activities is providing independence to learners means that the learners take the responsibility of their learning which in turn helps them in their capacity building. In such a situation, the syllabus is negotiated between learners and the teacher with – self-instruction, self-direction and individualization. It is therefore recommended that English learners must read extensively. The efforts of learners must be rewarded by the teachers so as to motivate their struggle to acquire the language skills. Government as a matter of priority should make available necessary facilities that will empower teaching and learning of English. Parents should arouse the interest of their wards by providing needed materials and conducive to learning and studying environment at homes.

REFERENCES

1. Gardner, Howard (2008), Five Minds for the Future. Boston, Massachusetts: Harvard Business School Publishing.
2. Government of India (2012), Twelfth Five Year Plan. Available at: http://planningcommission.gov.in/plans/planrel/12thplan/pdf/12fyp_vol3.pdf
3. National Curriculum Framework (2005), Position Paper: National Focus Group on the
4. Teaching of English (2006), New Delhi: NCERT.
5. National Curriculum Framework for Teacher Education (2009), New Delhi: NCTE.
6. Prabhu, N. S. (1982), The Communicational Teaching Project, South India. Madras: The British Council (mimeo).
7. Walker, D. F. and J. Schaffarzick (1974), 'Comparing curricula.' Review of Educational Research 44:83-111.
8. Davies, Allan and Beretta, Allan (1985), Evaluation of the Bangalore Project, Article in ELT Journal. Available at DOI: 10.1093/elt/39.2.121 · Source: OAI
9. Rachna, 2017. Teaching/Learning English of India: Challenges and Opportunities, UGC approved Journal No. 48520, ISSN 2454-3454, Vol.3, Issue 6, Nov-Dec 2017.
10. Mittal, Reena, (2014), International Journal of Research (IJR) Vol-1, Issue-7, ISSN 2348-6848 Emerging Trends in English Language Teaching
11. Rogers, E. M. (1983), The diffusion of innovations, 3rd ed. London and New York: MacMillan and Free Press.
12. OECD (2016), Innovating Education and Educating for Innovation: The Power of Digital Technologies and Skills, OECD Publishing, Paris.
13. Service English programme design and opportunity cost. (1989), In R.K. Johnson (ed.) The second language curriculum. Cambridge: Cambridge University Press. 79-90.
14. Kennedy, C. (1988), Evaluation of the management of change in ELT projects. Applied Linguistics. 9.329-342.
15. Havelock, R. G. (1971), The utilization of educational research and development. British Journal of Educational Technology. 2.84-97.., vol. 3, no. 2, **(2003)**, pp. 75-80.

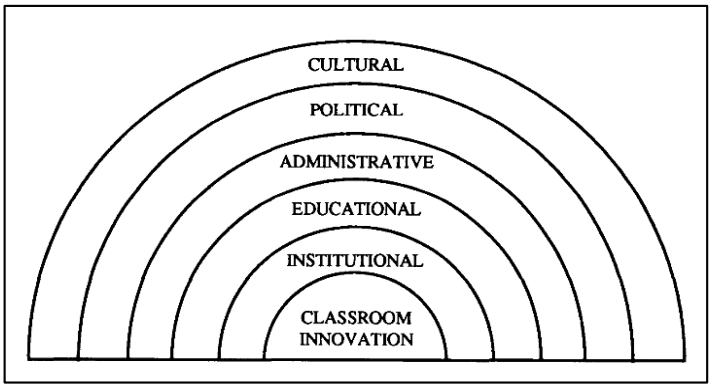

Figure 1. The hierarchy of interrelating subsystems in which an innovation has to operate (Kennedy, 1988).

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RESEARCH ARTICLE

Bioconversion of Rice Waste into Organic Manure through Vermicomposting using *Eisenia foetida*

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ABSTRACT

Bioconversion of organic wastes produced from various sources due to the activity of human highly need to manage by using vermitechnology for eco-friendly environment, sustainable agriculture and soil amendment with high nutrient supplement. Out of several wastes the cooked food wastes that produce from canteen, restaurant, hostels, industries, hotels, domestic kitchen and from various organized gatherings etc. Rice is mostly considered as a source in diet but also produced as a major organic waste after sufficient consume for it's preparation in large amount comparable to other items. Hence it is highly essential for safe disposal and management against food waste by creating awareness. Vermicomposting is a simple biotechnology process of composting where earthworms are used to enhance the process of waste degradation for production of organic manure as a better end product known as vermicompost. In this present study, the main focus was on the role of earthworm that converting the rice waste nutrients into a valuable composting product for agriculture utilization. The experiment was carried out for 60-80days by taking various proportions of cooked rice waste such as C (Control), R1, R2, R3, R4 and Expt. (Experimental) mixed along with cow dung and soil. The earthworm species Eisenia foetida was used in all proportion for the process of vermicomposting and obtained vermicompost as end product in R1 and R2. The physico-chemical parameters pH, electro conductivity, temperature and moisture content were analyzed in different time intervals to estimate the survivability, population growth etc. are key indicators for production of vermicompost.

Keywords: Vermicomposting, earthworm, Eisenia foetida, Rice waste (Rw)

INTRODUCTION

Food waste is also carrying credential for serious environmental issues caused due to growing population and demand of their living style. Approximately one third of food is produced from the human need according to the Food and Agriculture Organization (FAO) of UN and about 40% of food is produced from India (UN). The cooked food wastes are one of the major source for whole food waste considered as solid waste are generated from various source like canteen, restaurant, hostels, industries, hotels, domestic kitchen and from various organized occasions etc. Although the production of food waste has been carried out for fulfillment of human need but proper management, safe disposal and awareness for saving food are the major guideline to be followed in time for reduction of it. It is required to treat the food waste effectively in such a manner that should not generate environmental pollution and badly produce fouling smell that cause harmful health diseases. The best way to treat organic waste instead of disposal is vermicomposting which converts it into useful organic manure for sustainable plant growth ([2], [12]).

Vermicomposting is a biological treatment leading for degradation and stabilization of organic matter by the coactions of earthworms and microorganisms is considered as a mesophilic aerobic process. There are more than 3000 species of earthworms are recognized in the world that perform particularly in vermicomposting ([5], [7], [14], [15]). Vermicomposting has the major advantage compared to conventional compost such as odorless, adjusted pH, low electrical conductivity, and contains high concentration of elements such as nitrogen, potassium, and phosphorus ([3], [8], [11]). Vermicompost is stable and has uniform combination and level of contamination is less than raw materials and other fertilizers. Production of organic acids during process and presence of micronutrients such as iron, copper, and zinc in the vermicompost make it's effective fertilizer for plants. The organic acids, digestive tract secretions, exudates from the surface of worms ([5] ,[8]).

Granulated excreta of the worm is vermicasts has a bulk condition during vermicomposting, have a less density than usual compost, makes more porosity of soils and increases the permeability of water in soil. Presence of high humidity retention capacity in the vermicompost facilitate to carry water for longer period in plants ([3], [7], [16], [17]). Microbial activities improve nutrient status, microbial biomass carbon and enzymatic activities. Role of vermicompost in nourishing agricultural crops has attracted to the researchers throughout the globe. There is an increasing interest in the potential use of vermicompost as soil amendment, where the addition of vermicompost improves the soil physical and chemical properties. Bioconversion of rice waste can be possible using vermicomposting as a potential tool for ([18], [19], [20]). However, it is suggested that the rice waste can be amended with mixture of organic manure to ensure better quality of vermicompost [4]. The main objective of the study was to investigate the ability of rice waste to produce vermicompost by the action of *Eisenia foetida*.

MATERIALS AND METHODS

Experimental location

This experiment was carried out for about 3 months from January to March in the Laboratory of Department of Zoology, Centurion University of Technology and Management, located at Jatni, Bhubaneswar, Odisha, India.

Collection of Materials

The samples for present experiment were collected from various areas inside the campus of CUTM such as
--Fresh cattle dung-from cattle shade
--Soil-from garden area
--Rice waste-from canteen of hostels
--Earth worms (Eisenia foetida)-vermicomposting unit

Methods

The experiment was conducted to find out the production of vermicompost from rice waste by using it as best source of bedding material in vermicomposting providing nutrition for earthworm *Eisenia foetida*. The collected cattle dung and soil was allowed to dry for 7-8 days and then crushed and sieved to get fine material segregating from uncrushed one. The collected rice waste was settled for composting upto 7 days adding equal amount of fresh cattle dung. Various proportions of sieved cattle dung (Cd) and soil(S) including composting rice waste (Rw) were prepared by weighing in ratio of Cd+S (1:1) Cd+S-Rw(2:2:1), Cd+S-Rw(1.5:1.5:2), Cd+S-Rw(1:1:3), Cd+S-Rw (0.5:0.5:4) and 100% of cattle dung labelled as Control(C) ,R1, R2, R3, R4, Experimental (Expt.) respectively in 6 rectangular plastic pots.

Then the waste material as Rw were well mixed in the 6 pots with respective ratio of cattle dung and soil allowed for pre-composting upto 4-5 days. In the next procedure the collected earthworm specis *Eisenia foetida* were released as 3 in number into each container bearing a range of length from 7.5-10 cm after preparing the vermibed by using pre-composting. The whole set of proportion were proceeded with vermicomposting by regularly spraying water on the bed and adding slurry of cattle dung to it for maintaining moisture and nutrition along with rice waste. About one to two grams of samples were collected from each container for chemical testing in the mentioned lab before and after introducing of earthworms during the process of vermicomposting. The pots were covered by the nylon net to avoid the earthworm from danger predators, direct sunlight and were observed daily in order to check the various physico-chemical parameters, survivability, growth, population rate and formation of vermicompost.

METHODOLOGY

This experiment was conducted in two parts in the study i.e. the first part was pre-composting experiment and the second phase about entire procedure of vermicomposting where all major required parameters were measured to estimate. Different observations were carried by measuring the required physico-chemical parameter in a regular interval of every 15 days [19]. Similarly growth and population of earthworm Eisenia foetida in each pots were calculated in respect to their survival rate. The chemical composition of raw materials were detected by XRF. The vermicompost was the end product obtained from each pot determined by it's colour. Statistical analysis was carried out of these values to determine through mean and standard deviation (SD).

RESULT AND DISCUSSION

The present study was experimented out with cooked rice waste that was used, subsequently degraded and consumed by the action of both microbes and earthworm respectively in vermibed. The ultimate result was obtained as end product vermicompost with enriched organic nutrient for plant growth. The entire procedure of vermicomposting was conducted for 60-80 days and controlled by the maintenance of physico-chemical parameters like moisture content, pH and electro-conductivity. Analysis of all parameter values were tabulated and plotted in Table 2. And Figs. (1,2, 3 & 4). The findings of all parameters were varies for each proportion that estimated through mean and SD values. Out of whole the result was effective in R1 and R2 as compared to other with the standard proportion taken as Control(C).

The muscular grinding organ gizzard of earthworm Eisenia foetida consumed rapidly the rice waste and released dark black granular vermicast [9] later obtained as vermicompost (Table 3.). The survivability and growth of earthworm was observed more suitable in R1 and R2. However it was observed less number in R3 but almost nil in R4 and experimental after 20 days due to rapid microbial fermentation in more quantity of rice waste (Rw) from the pre-composting to till initial stage of undergoing process of vermicomposting. The fermentation converted each proportion into acidic medium initially then changed to slightly acidic [1] and it increased in respect to percentage of Rw. The pH in waste proportions was ranged from 5.2 to 6.8 which indicated that the acidification was more in R3,

R4, and Expt. May be caused due to nitrification of microbes (Table 2. and Fig.2) [21] .Similarly moisture content was maintained within 65%-75%. In R4 and Expt. contained more amount of water above than survival of Eisenia foetida initially due to degradation of waste that released water and later reduced Table 2. and Fig.3. The mineral salts added to vermibed due to the pre-composting which was available as nutrition for earthworm was detected by electro-conductivity (EC) (Table 2. and Fig.1). It was increased initially but later reduced due to conversion of salts found suitable in R1 and R2 [10]. The temperature was above 350C during pre-composting and early stage of vermicomposting due to generation of heat for decomposition of wastes which was later came down. The temperature was observed suitable in R1 and R2 as compared to others aid for survival of earthworm [6] (Table 2. and Fig.4) [6].Production of juveniles subjected to population growth for the chance of survival and growth of parent earthworm species Eisenia foetida (Table 1.).From above analysis of different parameters it was observed that rice waste nutrient plays important role in vermicomposting in low percentage upto 40% in vermimixture while increased in percentage caused decline in population indicated unsurvivable of earthworm. The growth of earthworm population is directly proportional to formation of vermicompost indicated to R1and R2 with Control due to all favourable parameters.

CONCLUSION

From the present study the chemical parameters of vermicompost at different time intervals of rice waste indicated the possibility of production is in less proportion including soil and cattle dung. The major proportion of rice waste causes acidification unable for earthworm survivability. But the effective output of present study can be a good practice to reduce volume of rice waste by using vermicomposting technique for production of eco-friendly and cost effective organic manure to utilize in agricultural field for sustainable cultivation.

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REFERENCES

1. R Jadhav, M..P. Chitanand and , H.G. Shete, “Flower Waste Degradation Using Microbial Consortium. Journal of Agricultural and Veterinary Science”, 3(5), (2013), pp 1-4.
2. C.A. Edwards, P..J. Bohlen, “Biology and ecology of earthworm”. 3rd ed. London: Chapman and Hall; (1996), p. 42.
3. G.R. Bachman, J.D. Metzger, “Growth of bedding plants in commercial potting substrate amended with vermicompost”. Bioresour Technol. (2008);99: 3155–61.
4. H. Deka, S. Deka, C.K. Baruah, J. Das, S. Hoque, N.S. Sarma “Vermicomposting of distillation waste of citronella plant (Cymbopogon winterianus Jowitt.) employing Eudrilus eugeniae”. Bioresour Technol. 102: ,(2011), pp6944–5.
5. J.M. Bremner, R.G. Mulvaney, Nitrogen-total. In: Page AL, Miler RH, Keeney DR, editors. “Methods of soil analysis. Part 2”. American Society of Agronomy, Madison, Wisconsin, USA. (1982). pp. 595–624.
6. L.B. Taiwo, and B.A. Oso “Influence of composting techniques on microbial succession, temperature and pH in a composting municipal solid waste”. *African Journal of Biotechnology*.;3(4),(2004), pp239-243 .

7. M. Ali, A Bhatia , A.A. Kazmi and N. Ahmed "Characterization of high rate composting of vegetable market waste using Fourier transform-infrared (FT-IR) and thermal studies in three different seasons". Biodegradation. (2012); 23: 231–42.
8. M. Chikae, R. Ikeda, K. Kerman , Y. Morita , E.Tamiya,. "Estimation of maturity of compost from food wastes and agro-residues by multiple regression analysis". Bioresour Technol. 97, (2006), pp1979–85.
9. M. Lakshmi Prabha,., M. Shanmuga, R. Priya, Pavithra., "Microorganisms in the Gut of Earthworm Eudrilus eugeniae". Int J. Curr. Res. Chem. Pharma.Sci),1(3), .(2014), pp 6-9.
10. N. Jain, Waste management of temple floral offerings by vermicomposting and its effect on soil and plant growth, International Jounal of Environment and Agriculture Research.,2(7), (2016) pp 2454-1850.
11. S. Adhikary, "Vermicompost the story of organic gold: A review. *Agricultural Sciences"*. 201203. 905-917. DOI:10.4236/as.(2012).37110.
12. S.A. Bhat, J. Singh , A.P. Vig,, "Vermiremediation of dyeing sludge from textile mill with the help of exotic earthworm Eisenia foetida Savigny". Environ Sci Pollut Res. (2013);20: 5975–82.
13. S.A. Bhat, J. Singh, A.P. Vig,, "Genotoxic assessment and optimization of pressmud with the help of exotic earthworm Eisenia foetida". Environ Sci Pollut Res.(2014); 21: 8112–23.
14. S.A. Bhat, J. Singh , A.P. Vig, "Potential utilization of bagasse as feed material for earthworm *Eisenia fetida* and production of vermicompost". Springerplus. (2015)a;4 :11.
15. S.A. Bhat, J. Singh, A.P. Vig, "Vermistabilization of sugar beet (Beta vulgaris L) waste produced from sugar factory using earthworm Eisenia fetida: genotoxic assessment by Allium cepa test". Environ Sci Pollut Res. (2015)b;22:11236–54
16. S.A. Bhat, S.S. Bhatti, J.Singh , V. Sambyal , A. Nagpal, A.P. Vig ."Vermiremediation and phytoremediation: eco approaches for soil stabilization". Austin Environ sci. (2016) a; 1(2):1006.
17. S.A. Bhat, J. Singh, A.P. Vig, "Effect on growth of earthworm and chemical parameters during vermicomposting of pressmud sludge mixed with cattle dung mixture". Procedia Environ Sci.b;35 (2016), 425–34.
18. S.A. Bhat, J. Singh, A.P. Vig, "Management of sugar industrial wastes through vermitechnology". Int Lett Nat Scic;55, . (2016). 35–43.
19. P. Campitelli , S. Ceppi, "Chemical, physical and biological compost and vermicompost characterization: a chemometric study". Chemometr Intell Lab. 90, (2008), pp 64–71.
20. S. Das, P. Deka, L. Goswami , B. Sahariah ,N. Hussain ,S,S. Bhattacharya. "Vermiremediation of toxic jute mill waste employing Metaphire posthuma". Environ Sci Pollut Res. (2016); doi:10.1007/s11356-016-6718-x.
21. Singh, Rajeev & Singh, Pooja & Araujo, et al. Management of urban solid waste: Vermicomposting a sustainable option. *Resources, Conservation and Recycling*. 55. 719-729. 10.1016/j.resconrec.(2011).02.005.

Table 1. Survival Number of Earthworm in Each Proportion during Vermicomposting

Sl No.	Proportional setup	Initial number of earthworms	Survival of earthworm in 1st 15days	Survival in 2nd15 days/ after1month	Survival in 3rd 15days	Survival in 4th 15days
1.	Control-C	3	6	10	15	22
2.	R1	3	5	9	13	19
3.	R-2	3	3	6	11	16
4.	R3	3	2	5	8	10
5.	R-4	3	1	death	death	death
6.	Expt.	3	1	death	death	death

Table 2. Measurement of Physio-Chemical Parameters of Various Observations during Vermicomposting

Sl. No	Observation	Electro-conductivity in S/m			PH			Moisture content			Temperature in ^{0}C	
		Initial	Final	Differ-ence	Initial	Final	Diffe rence	Before vermin composting	After vermin composting	Diffe rence	Initial	Final
1	C-100%	0.480	0.521	0.041	6.32	6.88	0.46	1.880	0.482	1.398	32.6	28.0
2	R1	0.523	0.498	0.025	6.11	6.76	0.65	1.481	0.384	0.997	30.8	28.2
3	R2	0.463	0.482	0.019	6.09	6.68	0.59	1.401	0.615	0.986	31.7	28.4
4	R3	0.460	0.488	0.028	5.92	5.21	0.71	1.348	0.5	0.848	30.6	29.1
5	R4	0.541	0.498	0.043	5.48	5.22	0.26	1.289	0.253	1.036	31.6	34
6	Expt.	0.495	0.517	0.032	5.64	6.32	0.68	1.410	0.418	0.992	32.3	34.7

Table 3. Colour and odour of vermicompost in all proportions after completion of vermicompoting

1	Control	Dark brown	Odourless
2	F1	Black	Odourless
3	F2	Black	Odourless
4	F3	Black	Odourless
5	F4	Greyish Black	Not obtained
6	Experimental	Grey	Not obtained

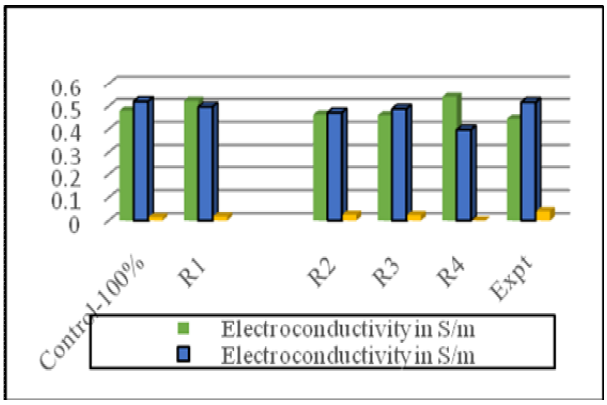

Figure 1. Graphical Presentation of Electro-conductivity of Each Rice Proportion

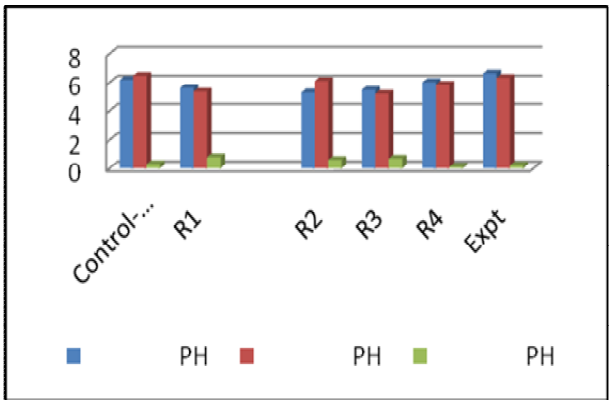

Figure 2. Graphical Presentation of pH of Each Proportion

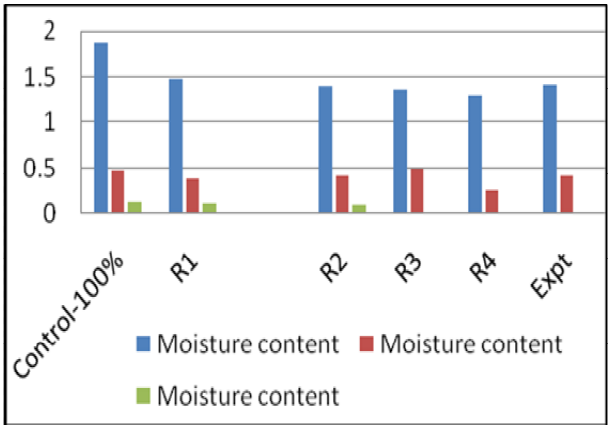

Figure 3. Graphical Presentation of Moisture content of Each Proportion

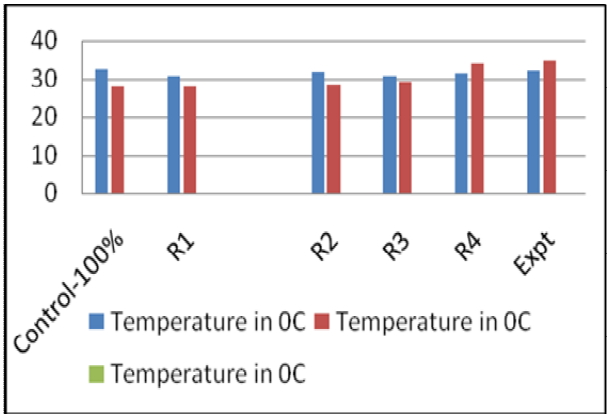

Figure 4. Graphical Presentation of Temperature of Each Proportion

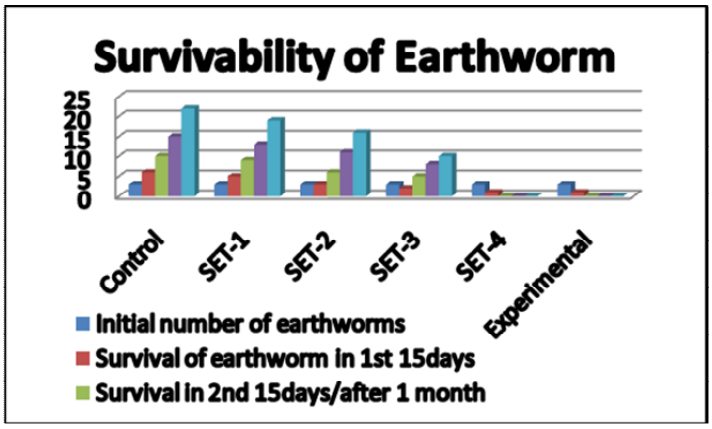

Figure.5 Graphical presentation of survivability of E arthworm

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RESEARCH ARTICLE

Taxonomical Identification of Vermicomposting Earthworm Species

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ABSTRACT

The biological indicator or biological manipulator are otherwise named for earthworms that has significant role towards the proper functioning of ecosystem and are economically and environmentally beneficial to the other soil organisms. Earthworms are soil dwelling organisms enhance the vegetation growth in an eco-friendly manner among other benefits as source of minerals, nutrition and enzymatic action adding to soil property. The diversity of earthworms varies across different parts of the globe and species identification is a key to specific regions according to their morphological and anatomical features The present study was conducted during the year 2019- 2020 at Centurion University of technology & Management, BBSR, Odisha, India. Samples of earthworms are collected 3-4 in number from the CUTM garden by utilizing the hand sorting method. The area is moist and showed rich in organic composition from where the earthworms are collected. The samples of earthworms were placed into a vermin-container. Taxonomic studies were conducted on the collected species in the laboratory. The morphometric and anatomical data were carefully examined based on the literature survey and the species was identified grouped into the family Eudrilidae.

Keywords: Vermicomposting, Eudrlidae, Morphometric features

INTRODUCTION

The earthworms has significant role in soil mechanism that enhance physical, chemical and biological properties of soil for large scale production of crops. Earthworm is a terrestrial annelid belongs to class Oligochaeta especially to family Lumbricidae of numerous widely distributed hermaphroditic worms that move through the soil by means of

setae and feed on decaying organic matter ([3], [6], [10], [16]). Earthworms are characterised as "contemplate" that they shift through whatever surrounds by turning, exploring and move through it. They lives in dark and moist place are conscious creatures with no great hurry but always in motion, shrinking and contracting, twisting and burrowing and consuming [7]. They spend their lives act on the detritus substances and particles of soil by consuming to form humus soil. Earthworms are cold-blooded due to moist in nature remain cool like humans sweating Earthworm is described as the 'unheralded soldiers of mankind [2] and the intestine of earth according to Aristotle the restoring agents of soil fertility [1]. Earthworms are biological indicators of soil quality [16, 17]. It is allowing water and air to reach plant roots and improving soil conditions for beneficial bacteria and micro – organisms for their burrowing habit.

The physiological processes of earthworm are controlled such as breathing process is occur through their skins due to the osmosis process i.e oxygen is entered to the circulatory system through the body wall. A film of mucus layer is covered the skin of earthworms which provides to hold moisture and lubricates during dwelling process in the soil. The walls of burrows is sealed by secretory mucus and is also important for reproductive process ([4], [5]). Earthworms have been survived for millions of years possesses a streamlined body to move beneath the ground. They do not possess eyes, ears or teeth or limbs either. They can react accordingly in senses, vibration, light and movement. Earthworms contains segments called somites or annules are heavily muscled helps in easy locomotion, bourrowing and found more in number in larger worms than smaller ones [8]. There are tiny bristles called setae are present in each segment, and these help the worm to move, to stay put in the ground from predator and help the worm while mating [18].Worms bear five "hearts", which helps in blood flows through two major blood vessels that run on the top and the bottom of the worm's body.

There are about 70,000 species of earthworms are present in the soil everywhere except desert and arctic regions throughout the world. In the Middle East, Europe, and Asia, the earthworm species were originated and later have been since introduced to the Americas and islands. Earthworms are widely known with various names such as Lumbricus, Lob worm, angleworm, fishing worm, Nightwalker, dew worm and Red worm. [11]. Earthworms are categorized in to three major groups on the basis of their burrowing and feeding habits such as: 1) Endogeic :-Worms are are medium-sized and pale in color live in the upper layers of soil in the Rhizosphere region. It shows better aerating and moisture holding for soil. 2) Anecic:-Worms live in deep burrows on at day time and come to surface in night, hence night crawler and fed on decaying matter [13] and 3) Epigeic:- Worms live in loose organic litter not in burrow are surface dwellers, feed on decaying matter and it's casting is more in nutrition than other type . But all play important roles in the soil food web [20].

There are several species of earthworms are present in the world such as Eisenia foetida, Lumbricus rubella, Pheretima posthuma, Eudrilus eugenie, Perionyx excavates, Lempita mauritii etc.. Most of the species are use in the vermicomposting process. Vermicomposting is a natural nutrientrich, microbiologically active organic amendment process that results from the interactions between earthworms and microorganism during the break down of organic waste that convert into vermicompost. The present taxonomical study focus on to identify the collected earthworm species that potentially involved in vermicomposting.

MATERIALS AND METHODS

Collection of Materials

In this study, four-six earthworms were collected in a container from vermicomposting unit of CUTM campus of a species. Only the adult earthworm of the species was collected for better identification.

Method

The collected earthworm were washed and cleaned in running tap water and then preserved in a mixture of 1.5 ml of formalin and 100ml of water in a container. After that standard method is followed for morphological and anatomical features of earthworm were carried out in the laboratory of Zoology Department, CUTM, Odisha, India.

RESULT ANALYSIS

In the present taxonomical study of earthworms was carried out by it's morphological and anatomical features referred to literature survey with it's body colour, clitellum position, somite etc. and soil types. Result of the morphological study of earthworm species of CUTM garden was obtained with the color of anterior portion of the earthworm is purplish red worm and posterior portion is dark brown color. The length of the earthworm is approximately ranges from 15cm to 19 cm and diameter is 4-6mm. There are approximately 198-217 number of rings are present in the earthworm. The position of clitellum is present found in segment XIV, XV, XVI. The male pore found in XVII/ XVIII segment and female pore in XIV. Prostomium or mouth is present in the segment I. The result from anatomical study of the earthworm species showed that esophagus is extending in the segments V-VIII. Gizzard which grinding the food particles present in the segment IX, X, XI. The origin of the intestine from the segment XIV/XV to till end. The Dorsal blood vessels is in segments VII -XIV, Heart is 7 in number on the lateral side of body which is present in segment VI, VII, VIII,IX.. Due to the above studied the collected earthworm species is identified from literature survey belongs to the family Eudrilidae and the species is Eudrilus eugeniae [9] which is best for the vermicomposting process.

DISCUSSION

The above observations of earthworm species was studied and identified the morphological characteristics from body size clitellum and genital pore. The environment is inhabited by most earthworms were quite stable and these determined the time it takes to mature in some species ([9], [15]). All the earthworms were sexually mature at the time of collection as showed by the presence of the clitellum and lived in large amount of decaying materials adopted varied environmental except extreme heat [12]. All the resulted characteristic were matched with volumes of literature survey for their dichotomous key and the above morphological and anatomical features are present in the species which identified as Eudrilus eugeniae (Taxonomy follows the codes and conventions of Blakemore) ([13], [15]). Due to the above studied the collected earthworm species is belongs to the family Eudrilidae and the species is Eudrilus eugeniae which is best for the vermicomposting process. A survey was conducted in 2012/13 across different regions of Ethiopia to collect and identify suitable species of earthworms to develop for vermiculture .E. eugeniae earthworm were isolated as the best earthworm for vermicomposting from the collected worms. This earthworm also called as Night crawler which is native to tropical West Africa and now wide spread in warm regions under vermicompost, this worm is an excellent source of protein and has great pharmaceutical potential.

CONCLUSION

From this present taxonomical study it was carefully observed and statistically analyzed certain characteristics of the collected species that identified as Eudrillus eugeniae resembles approximately with the characteristics that reported from literatures ([11], [21]) and simplified key to common genera of terrestrial earthworm with following characters

Domain –Eukarya(true nucleus with membrane bound organelles)
Kingdom -Animalia(Multicllular,heterotrophic)

Phylum	–Annelida(Annules present throughout entire body)
Class	- Clitellata (presence of prominent clitellum)
Sub-Class	- Oligochaetae (Setae located ventrally, laterally or dorsolaterally,hermaphrodite)
Order	- Heplotaxida (Male pore at 17-18 segments)
Family	- Eudrilidae (Sadle shaped clitellium ranges-9-12 segments, Gizzard at 17-19 segments)
Genus	-*Eudrilus* (Kinberg,1867 [9]-reported-African night crawler, epigeic)
Species	-*Eudrilus eugeniae* (Blakemore, 2012)

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REFERENCES

1. A.E. Shipley, "In:The Cambridge Natural History" (Harmer, S. F. and Shipley, A. E. eds.). Codicote, England, (1970).
2. C.R. Darwin, "The formation of vegetable mould through the action of worms with observation on their habits. Murray", London,(1881).
3. C.A. Edwards and J.R. Lofty, "Biology of Earthworms. Chapman and Hall", London, (1972).
4. C.A. Edwards, and P.J. Boglen, "Biology and Ecology of earthworms", 3rd Edition, Chapman and Hall publication, 2-6 Boundary Row London, UK, (1996), 202-217.
5. D. Krogh, " Biology: A guide to the Natural" World. 3rd ed. Prentice, (2005).
6. F.Koch, et al, "Genome-wide RNA polymerase II: not genes only! Trends Biochem Sci" 33(6): (2008) 265-73.
7. G.H. Basker, "Penggunaan pelapis lunak untuk mengurangi rasa sakit pada alveolar ridge yang tajam" E-Journal Wicya Kasahatan Dan Lingkungan vol-1--(1993)No-1-2014.
8. J.C. Blackburn, "External anatomy of earthworms". Sci. 207, 1989, 2572 – 2577.
9. J.G.H. Kinberg, "Annulata nova.Ofersigt of Kungliga Svenska Vetnskaps-Akademiens Forhandlingar" 1866, Stockholm (1867)23(4):97-103.
10. J.M. Julka, R. Paliwal, P. Kathireswari, "Biodiversity of India earthworms-an overview". Proceedings of Indo-US Workshop on Vermitechnology in Human Welfare. Rohini Achagam, Coimbatore, (2009) pp: 36-56.
11. Pirrone, "The earthworm baits market in North America. Heredity" Nature and Science, 5(2), 2007, B.O. Oboh, D.O. Akintobi and C. Ejidereonwu, Morphometric studies in Eudrilus eugeniae populations from different locations in Lagos, Nigeria 21. 59: (1985) -1019 – 1029. 20 .
12. P.S. Chaudhuri, K Pal, G Bhattacharjee and S.K. Dey "Chemical changes during vermicomposting (Perionyx excavatus) of kitchen wastes". Trop.Ecol41, (2002), 107-110.
13. R.J. Blakemore, "Eco-taxonomic profile of the iconic vermicomposter - the 'African Nightcrawler', Eudrilus eugeniae (Kinberg, 1867)". African Invertebrates 56: 527-548. Archived from the original on 2016-10-22.
14. Robert J. Blakemore, "Eco-Taxonomic Profile of an Iconic Vermicomposter — the 'African Nightcrawler' Earthworm,Eudrilus eugeniae(Kinberg, 1867)". African Invertebrates. **56** (3): 527–548.-(2015)., doi:10.5733/afin.056.0302.
15. S.A. Ismail, "Vermicology: The biology of earthworms". Orient Longman Press, Hyderabad, (1997). p92 .
16. S.A Ismail, "Organic waste management. In: Technology Appreciation Programme on Evaluation of Biotechnological Approaches to Waste Management" held on 26th October 2000. Industrial Association-ship of IIT, Madras, (2000). pp. 28–30

17. S., Kramer, et al."Reduced nitrate leaching and enhanced denitrifier ativity and efficiency in organically fertilized soils. Biological Sciences - Ecology - Biological Sciences - Sustainability Science" 103, (2006) 4522-4527.
18. GarryOakEcosystem(GOE):https://www.canadianfieldnaturalist.ca/index.php/cfn/article/view/113
19. Silva, A. Pathiratne, A.M. Cornelis, V. Gestel, "Toxicity of Chlorpyrifos, Carbofuran, Mancozeb and their formulations to the earthworm Perionyx excavates". In Thesis 2009–2004 of the department of ecological science, Amsterdam: VU University (2009)

Table 1. Tabulation on Morphological Characteristics

Slno.	Observ-Ations	Species	Length (In Cm)	Diam-Eter(In Cm)	Body Weig-Ht (In Gm)	Prost omiu m	Femal Pore	Male Pore	Clitellu m	Body Segm -Ent
1.	1st	*E.eugineae*	15.2	0.4	2.32	Epilo bous	14^{th}	$17/18^{th}$ segment	14 to 16	198
2.	2nd	*E.eugineae*	17.2	0.6	3.17	Epilo bous	14^{th}	$17/18^{th}$ Segment	14 to 16	211
3.	3rd	*E.eugineae*	18.7	0.4	3.42	Epilo bous	14^{th}	$17/18^{th}$, segment	14 to 16	217
4.	4th	*E.eugineae*	16.7	0.6	2.61	Epilo bous	14^{th}	$17/18^{th}$ segment	14 to 16	208
5.	5th	*E.eugineae*	16.1	0.4	2.67	Epilo bous	14^{th}	$17/18^{th}$ segment	14 to 16	206

Table 2. Tabulation on Anatomical Characteristics

Sl.NO.	Observ -ations	SPECIES	Pharynx position in sgmnt	Gizzard position in segment	Oesophagus position in segment	Intenstine position in segment	No. of Hearts
1.	1st	*E.eugineae*	2-3	9-11	5-8	14/15- end before last 5-6 segments	7
2.	2nd	*E.eugineae*	2-3	9-11	5-8	14/15- end before last 5-6 segments	7
3.	3rd	*E.eugineae*	2-3	9-11	5-8	14/15- end before last 5-6 segments	7
4.	4th	*E.eugineae*	2-3	9-11	5-8	14/15- end before last 5-6 segments	7
5.	5th	*E.eugineae*	2-3	9-11	5-8	14/15- end before last 5-6 segments	7

AUTHORS

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RESEARCH ARTICLE

Bioconversion of Dry Leaf Litter of Cadamba (*Anthocephalus indicus*) tree into Vermicompost by the Action of Earthworm (*Eudrilus eugeniae*) for Sustainable Plant Growth

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ABSTRACT

Disposal of waste is a universal problem. Available methods require manpower, lot of money and area to manage waste. Plant generating waste is a type of organic waste which can be use better for soil reveal changes in physical factors during vermicomposting and also vermiculture. The objective of the present study is to find the possibility of utilization of Cadamba (*Anthocephalus indicus*) leaf litter from the campus of Centurion University of Technology and Management, Odisha, India through vermicomposting by increasing the population of vermireactor Eudrillus eugeniae in the process of vermiculture. It is at least a century years old but it is now used worldwide for the management of waste substances. The earthworm increases nutrient availability, better drainage, and more stable soil structure. Higher feeding, growth and biodegradation capacity in soil was found in the species E. eugeniae. Enhancement in natural biodegradation and decomposition of wastes was shown by the action of earthworm within 70-80days.The degradation of all the waste were taken in the study achieved with increasing in physical growth as well as population growth of the earthworm after consumption as nutrition. Earthworm eject humus rich casting and form water stable aggregates which improves soil physical and chemical properties. Casting also contains enzyme like protease, amylase, lipase, cellulose and chitinase to decompose organic matter. The action of earthworm in vermicomposting is by physical and biochemical process. The present paper gives the information on role of earthworm in vermicomposting and vermiculture. In recent years the vermicomposting process has attracted researchers for environmentally sound treatment of wastes. The main objective of the present work was to evaluate the potential of earthworm on conversion of leaf waste into vermicompost for utilizing plant growth. .

Keywords: Cadamba (*Anthocephalus indicus*) leaf litter, pH temperature, moisture, biomass reduction

INTRODUCTION

Generation of leaf litters from the tree planted in public as well as private places is a major problem in term of their disposal [1]. Conventional methods of amputation viz. burning, dumping not only make the environment polluted but it also affect the health of human being [2]. Bio-organic waste required efficient way to sustain ecological temperament as well as improve natural resources [5]. Composting is the splendid approach to resolve generated bio waste. It is an aerobic or anaerobic process involving several micro flora viz. bacteria, fungi and actinomycetes that assist in breakdown of organic matter to nutrient like compound humus [22]. Composting has numerous benefits but a few limitation requisite additional approaches to accomplish the demand. Vermicomposting is an improved part of composting but it differs from composting in several ways and it also faster than composting ([6],[7]). It is the result of combined activity of microorganisms and earthworms in which primary decomposition take place outside while secondary decomposition takes place inside the earthworm [22]. Researchers have been put their efforts in recycling of different type of waste like sewage sludge, animal wastes, crop residues, industrial wastes etc. by using vermicomposting ([13], [16], [18]) in recent years. Leaf litter is a byproduct of agriculture also processed through earthworm ([19], [20]). The production of vermicompost from different leaf litters such as wheat straw [8] , Sugarcane leaf [15], Ashoka tree leaf litter (Polyalthialongifolia), Teak tree leaves litter (Tectonagrandis) and Neem tree leaf litter (Azadirachtaindica) [3] , Tendu leaf litter [11], Mango and Guava leaf [10] , Rubber leaf litter [21] , Teak leaf litter [17], Eucalyptus [19] , have been reported so far. Out of several leaf litters Cadamba is a well known ornamental tree produce huge in quantity.

The botanically known as *Anthocephalus indicus* and scientificaly name as *Neolamarckia cadamba* belongs to the Rubiaceae . It is an economical plants used for preparation of perfumes, timber, paper-making, medicine, worship etc. It is significantly produce largest number of phytochemicals and secondary metabolites having pharmacological and biological properties that can be used prevention as well as the treatment of several incurable diseases. The Cadamba is commonly known as “Cadambba” in Sanskrit and Hindi and as “Kodom” in Bengali. It is an evergreen tropical tree found in different parts of India, Bangladesh, Nepal, Myanmar, Sri Lanka, Cambodia, Laos, Philippines, Malaysia, Indonesia, Papua New Guinea, and Australia. Vermicomposting is a composting process using special species of earthworms usually Red Wigglers, Eudrilus eugeniae, Perionyx excavates, Lampiti mauriti etc. including other worms such as white worms and microbes to create a mixture utilizing decomposing dry leaf litter or solid waste breeding material etc. The breakdown of organic matter by earthworm produces vermicast as end product convert to vermicompost later. The biological, physical & chemical property of soil can enhance by adding of earthworm excreta as cast. Earthworms are physically aerator, crusher, mixture chemically degrader and biologically a stimulator in decomposition system[4]. Earthworms are terrestrial invertebrates belonging to the Order Oligochaeta, Class Chaetopoda, Phylum Annelida, which have originated about 600 million years ago, during the pre-Cambrian era [23]. Depending on factor like soil texture, aeration, pH of the soil, dung and litter, the earthworms are distributed and are burrowing animals that forms burrows in their way of feeding. Earthworms are not survive or rare in very coarse soil texture and high clay content or soil with pH 4 [9].

Earthworms are hermaphrodites but require another one to mate at clitellum region that produce cocoon. Two or more baby worms are hatched from one Cocoon. Production of Cocoon begins at the age of 6 week and continued till the 6 months. The incubation period of a cocoon roughly 3 to 5 weeks such as 3-30 weeks in case of temperate worm and 1-8 weeks in tropical worms. The incubation period varies among species. Vermiculture is an innovative sustainable method for mass production of the earthworms used in waste degradation and composting with vermicasts production can effectively manage the waste. The earthworm species Eudrilus eugeniae known as African night crawler is an excellent source of vermicomposting that has immense potency of biomass productions with releasing greatest number of cocoons in short period of time. The main objective of the present work is to

manage and recycle solid waste like dry leaf litter by using bioconversion procedure vermicomposting, with the activation and growth rate of earthworm related to various physico-chemical parameters.

MATERIALS AND METHOD

Collection of Materials

The present experimental study on vermiculture was carried out approximately about 80-120 days for the duration of November (2019) to February (2020) on the campus of CUTM, located at Jatni, Bhubaneswar, Odisha, India. Collection of materials soils, cow dung, dry leaf litter (Cadamb) were carried out from CUTM campus. The dry leaf litter (Cadamb) and soil was collected from the garden area of the CUTM campus whereas cow dung was collected in large-sized plastic containers from cattle shed of the CUTM campus. The earthworm species *Eudrilus eugeniae* was used for vermiculture collected from the vermiculture center of CUTM.

Method

The collected all the 3 material were allowed for drying, crushing and then sieving to segregate uncrushed one. The dried and sieved materials were used to weight for 6 different proportions labelled as Control (1:1), P1 (4:1), P2 (3:2), P3 (2:3), P4 (1:4), Experimental (100%) as experimental in 6 plastic similar pots. All the materials were thoroughly mixed and allowed with sprinkling of water upto contain proper moisture in all pots for pre-composting.

Process of Vermicomposting

The process of vermicomposting was started by introducing earthworms into the pot. Each pot was supplied by 3 earthworms *Eudrilus eugeniae* of various length. Water and cow dung slurry were added to the pots for regular maintaining of earthworms within time interval for their moisture content and room temperature. The earthworm *Eudrilus eugeniae* was not survived in S4 and experimental in initial stage but later adopted to produce population. After 15 days of monitoring the earthworms were observed with reproduce juveniles during consuming the waste with survive in the favorable condition. The earthworm *Eudrilus eugeniae* converted the waste into vermicompost after releasing of vermicasts. Regular sprinkling of water was carried out within 4-5 days of gap to maintain moisture regularly which is highly required for survival of earthworm. This process was carried out till the obtaining of vermicompost and stopped before harvesting. The final vermicompost of dry leaf litter was removed out in a separate container for plant cultivation and earthworms used in new vermicomposting pit.

Methodology

This present experiment was carried out in two phases i.e. the first part was pre-composting of collected raw materials and the second phase about vermicomposting after supplying earthworm into pots in respect to all major required parameters were measured to estimate [12]. Observations were carried by measuring required different physico-chemical parameter in a regular interval of every 15 days. Growth and population of earthworm used species *Eudrilus eugeniae* in each pots were calculated in respect to their survival rate. The chemical composition of raw materials were detected by XRF. Statistical analysis was carried out for all variables to determine through mean and standard deviation (SD). The vermicompost was the end product obtained from each pot was estimated by it's colour and were odorless.

Germination Study

Germination was done by sowing seeds of, *Cucurbita Maxima* into each pot having different proportions. Then the germination was appeared after 5 days and was observed upto 20 days (Table 4.)

RESULT AND DISCUSSION

Present study shows that odor of vermicomposting mixture was quite unpleasant during beginning days and it was gradually changed and finally turned into earthen smell. It was also found that mixture of leaf liter, cow dung was more stink than 100% cow dung. The hitting was found more in early phase of composting but later it turned down and finally temperature sets similar to room temperature. The colour of composting mixture was noticed and it was found light greenish yellow color at initial phase but at the time of maturation of vermicompost it turned into dark brown color (Table 5.). Like other waste, dry leaf litter (Cadamb) was used as an organic substrate with soil and cow dung in different proportions and especially it was treated as nutrition. During vermiculture the dry leaf litter (Cadamb) along with soil and cow dung was consumed and passing through gizzard later released vermicasts. The survival rate was increased depending upon the growth and capacity of reproduction due to physiochemical variables temperature, electro-conductivity, pH and water holding capacity (moisture content) were also observed as the following Table 1., 2., 3.) and Figures(1,2,3,4). Each proportion varies with their physico–chemical variables studied and observed with respect to electro conductivity, pH, temperature and moisture content. The pH value of each proportion mixed with dry leaf litter (Cadamb) powder in this experiment was ranged from 6.5 to 7.8 where the dry leaf litter Cadamb) mixture reduced the acidity of soil may due to presence of rich calcium .It was shown in Table-1 and Fig.1-1 that the slightly acidic soil when mixed with dry leaf litter (Cadamb) powder converted towards alkaline may be addition with cow dung during the process of vermicomposting with combining action of microbes and earthworms changed the pH towards alkaline within 7.5 which is suitable for survival of earthworm and plant growth [14]. The electro-conductivity was increased from the initial value during vermicomposting might have added salinity to each proportion due to composting of calcium carbonate of egg shell. The moisture content was slowly increased due to the physical action of earthworm in vermibed and the temperature was maintained below 35 ^{0}C that indicated the survival and enhanced the earthworm population (Table 6.) which yielded with faster vermicompost. The suitable vermiculture and later vermicompost rate was initially observed in P1 and P2 as compare to other due to less proportion of dry leaf litter. But subsequently it was obtained in all proportion with different time as per quantity of proportion. It was also shown in 100% dry leaf litter (Cadamb) proportion within 90-100 days. It was observed that in almost all proportion the population was achieved represented in (Table 6.) with production of vermicompost.

CONCLUSION

Plant leaf litter wastes have become additional source of pollution, foul smell unhygienic atmosphere and human health hazards. Their disposal and management is a big challenge to the government and administration.. Such nutrient rich wastes have possibilities to become the source of useful end product like compost. The purpose of present study is to find the way of vermicomposting of CADAMB leaf litter. With this study we can conclude that addition of cow dung with leaf litter and soil enhance the rate of decomposition. Addition of earthworm also improve the quality of final product. During vermicomposting we also analyzed different physical parameters viz. PH, temperature, moisture content and electro conductivity.

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REFERENCES

1. Aalok, A.K.Tripathi , "Composting- Vermicomposting of different types of leaves using earthworm species Eisenia fetida. Dynamic Soil," Dynamic Plant 4 (Special issue 1):, 2010,139-144.
2. A.K. Sannigrahi, "Management of some aquatic weeds through vermicomposting", Indian Journal of Environmental Protection, 29(9):(2009),809-811.
3. B.Jayanthi., G. Ambiga and P .Neelanarayanan ,"Utilization of mixed leaves litter for converting into vermicompost by using an epigeic earthworm Eudrilus eugeniae",.Nature Environment and Pollution Technology. 9(4), 2010, 763-766.
4. C.A. Edwards, P..J. Bohlen, "Biology and ecology of earthworm". 3rd ed. London: Chapman and Hall; **(1996),** p. 42.
5. G. Tripathi and P. Bhardwaj, "Earthworm Diversity And Habitat Preferences In Arid Regions Of Rajasthan",Zoos' Print Journal 19(7): (2004),1515-1519.
6. Gandhi M, Sangwan V, Kapoor KK and Dilbaghi N. 1997. Composting of household wastes with and without earthworms"
7. Environment and Ecology, 15(2):(1997) 432–434 .
8. Gandhi M, Sangwan V, Kapoor KK and Dilbaghi N. 1997,"Composting of household wastes with and without earthworms"Environment and Ecology, 15(2):(1997b) 432–434 .
9. Indrajeet and J.Singh, "Preparation of recipe for quality production of vermicompost. Journal of recent advances in applied sciences", (JRAAS) 25, (2010) 12-14.
10. K. Gunathilagraj, and T, Ravignanam , "Vermicomposting of sericultural wastes; Madras Agricultural Journal; Coimbatore, India"; ,(1996) pp. 455-457.
11. K Vasanthi., K Chairman., and A..J..A. Ranjit Singh, "Vermicomposting of leaf litter ensuing from the trees of Mango (Mangiferaindica) and Guava (Psidiumguujuvu) leaves", International Journal of Advanced Research. 1(3), (2013).33-38.
12. L.C. Mushan, and , K. R Rao,. "Physico-chemical analysis of tendu leaf litter vermicompost processed By Eudrilus eugeniae", DAV International Journal of Science 1(2), (2012), 100-102.
13. M.C. Dash, "Fundamentals of Ecology". Tata McGraw-Hill, New Delhi, India, (1993), pp. 210.
14. Mitchell MJ, Hornor SG, Abrams BI (1980). Decomposition of sewage sludge in drying beds and the potential role of the earthworm, Eisenia fetida. Journal of Environmental Quality 9: 37-378.
15. N. Jain, Waste management of temple floral offerings by vermicomposting and its effect on soil and plant growth, International Jounal of Environment and Agriculture Research.,2(7), **(2016)** pp 2454-1850.
16. P. Alagesan, and R. Dheeba, "Utilization of earthworms in organic waste management", Proceedings of the 15th International Forestry and Environment Symposium, (2010)., 26-27.
17. P.L.S Chan, D.A. Griaths, "The vermicomposting of pre-treated pig manure. Biological Wastes" 24: (1988). 57-69.
18. P. K. Nagalakshmi. and M. Prakash,. "A Microcosm Study of Cast and Gut of an epigeic earthworm *Perionyx ceylanensis* reared on different substrates**",** *Int. J. Curr. Trend. Pharmacobiol. Med. Sci.*1(2), (2016), 45-51.
19. R.Hartenstein , M.S. Bisesi , "Use of earthworm biotechnology for the management of effluents from intensively housed livestock". Outlook on Agriculture 18: (1989), 3-7.
20. R. Nagar, A.Titov and P. Bhati, "Vermicomposting of Leaf litters: Way to convert waste in to Best", INT J CURR SCI, 20(4): E 25-30, (2017), ISSN 2250-1770.
21. R. Nagar, A.Titov and P. Bhati, "Vermicomposting of green Eucalyptus leaf litter by Eisenia foetida and Eudrilus eugeniae" ",International Journal of Environment, Agriculture and Biotechnology (IJEAB), Vol-2, Issue-6, Nov-Dec- {2017) ISSN: 2456-1878.
22. S. Nath, and P.S. Chaudhuri, "Growth and reproduction of *Pontoscolex corethrurus*(Muller) with different experimental diets", *Tropical Ecology* .55(3), (2014).,305-312.
23. S.Shouche, P. Bhati , P. Pandey, "Study about the changes in physical parameters during vermicomposting of floral wastes", Journal of Environmental Research and Development 6(1): (2011).

24. T. G.Piearce,, K. Oates,. and W.J.Carruthers,."A fossil earthworm embryo (Oligochaeta) from beneath a late bronze age midden at Potterna, Wiltshire", UK. J. Zool. Land., 220: (1990),537-542.

Table 1. Measurement of pH and Temperature of each proportion

No of Reading	Name of Containers	Initial of pH	Final of pH	Temperature before vermicompost	Temperature after vermicompost
1	Control	6.78	6.89	23.4° C	26°C
2	P1	6.53	6.65	23.3°C	26°C
3	P2	6.36	6.45	23.2°C	26.2°C
4	P3	6.81	7.00		26.5°C
5	P4	7.07	6.88	23.2°C	27°C
6	Experimental	8.06	7.86	23.3°C	29°C

Table 2. Measurement of Moisture content of each proportion

No. Of Readings	Name of Pots	Weight of Wet Compost Soil	Weight of Dry compost Soil	Difference(moisture content)
1	Control	2gm	1.1363gm	0.8637gm
2	P1	2gm	1.0694gm	0.9706gm
3	P2	2gm	0.9391gm	1.0609gm
4	P3	2gm	0.8539gm	1.1461gm
5	P4	2gm	0.7914gm	1.2086gm
6	Experimental	2gm	0.639gm	1.361gm

Table 3.Observation of Germination (Pumpkin plant) duration & Plant growth

SL.No	Experimental Setup samples	Germination duration	Plant Growth Rate in cm Observation from 0-20 Days			
			0-5 Days	5-10 Days	10-15 Days	15-20 Days
1	Control	2 Days	3.2	8	17	26
2	P1	2 Days	3.1	7	16.5	22
3	P2	2 Days	3	6	15.2	20.8
4	P3	2 Days	2.7	6.2	11	18.7
5	P4	3 Days	2.3	5.4	9.3	16
6	Experimental	2 Days	5.1	11	18.2	28.6

Table 4. Colour and odour of vermicompost in all proportions after completion of vermicompoting

Sl.No.	Observations	Colour of vermicompost	Odour of vermicompost
1	Control	Dark brown	Odourless
2	F1	Black	Odourless
3	F2	Black	Odourless
4	F3	Black	Odourless
5	F4	Greyish Black	Not obtained
6	Experimental	Grey	Not obtained

Table 5.Observation survival and population growth during vermicomposting

Sl. No	Observations	Initial number Of Earthworm	Survival of earthworm in 15days	Survival in 30days/ after 1 month	Survival in 45days	Survival in 60days
1	Control	4	7	11	17	24
2	P1	4	6	10	19	25
3	P2	4	7	11	17	23
4	P3	4	5	9	14	22
5	P4	4	5	9	13	22
6	Experimental	4	4	5	7	13

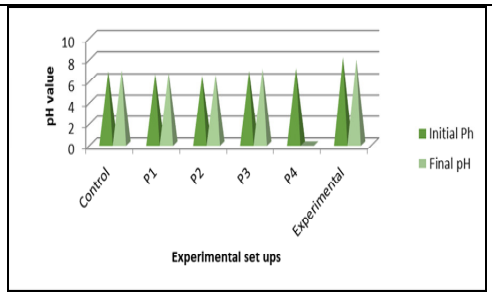

Figure 1. Mean of pH during vermicomposting

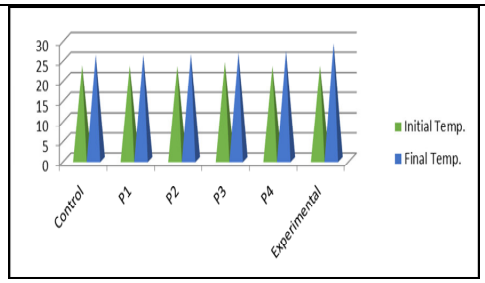

Figure 2. Mean of Temperature difference during vermicomposting

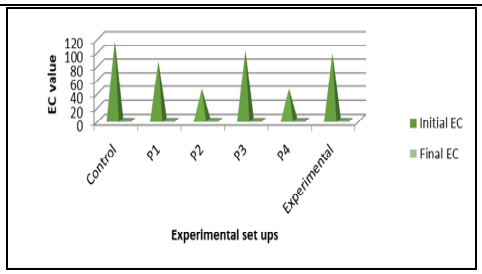

Figure 3. Mean of Electro-conductivity during Vermicomposting

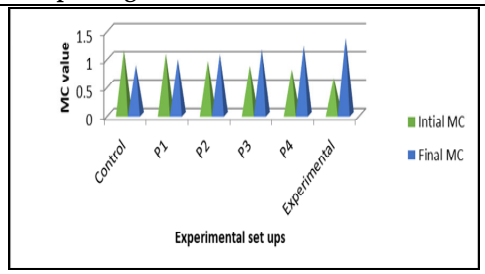

Figure 4. Mean of Moisture Content during vermicomposting

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RESEARCH ARTICLE

Laser Beam as an Optical Marker in Measurement of Bulk Diffusivity Coefficient of Sucrose

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ABSTRACT

Bulk diffusivity of aqueous sucrose solution in water is measured as a function of the mass concentration of the solution employing a recently developed "radial laser beam" marker technique [1]. The purpose of this study is to validate this technique as a general procedure for measuring the bulk diffusivity of any transparent solution diffusing into a transparent medium.

Keywords: Radial Laser Beam, Optical Marker

INTRODUCTION

Diffusivity measurement is fundamental to characterization of any mixing process where we need two or more materials to mix thoroughly. This measurement is also vital to industries like Metallurgy, Pharmaceuticals, Food Processing, Paints, Mining, Textiles, Cosmetics etc. However, there is no universal ab initio theoretical frame work which enables an accurate calculation of diffusivity D for any pair of materials A and B. Furthermore, with the compounding number of varied materials, which can be custom-mixed with each other to produce qualitatively new materials needed for various purposes, the importance and challenge of accurate measurement of D can never be overstated. The only possible recourse, therefore, is to measure this material property for a given pair of materials by an appropriate experimental design. The process of mixing is driven by the gradient of the concentration of the participating materials (both the A, the "solute" or "minor component" and B, the "solvent" or "major component"). Equivalently, the process can also be measured as a function of mass fraction of A in B.

The modern day techniques deployed to measure D include various methods in both Equilibrium and Non-equilibrium regimes as shown in the figure (1)[2]. As noted by Philibert [11], the results of the first attempt to measure diffusivity were reported by Thomas Graham in 1833. Adolf Fick thorugh his experiments (1855-56) coined the Laws now known in his name. The theoretical attempts to derive expressions for D were reported by Einstein (1905-1908) (now known as the Stokes-Einstein relation) and Smoluchowskii in 1906. They derived theoretical

expressions for *D* for various simple geometrical shapes of *A* against simple solvent *B* by considering the mean square displacement of molecules of *A* as a function of time *t*. These derivations were experimentally verified by Perrin and reported in 1909. However, the unlimited combinations of *A* and *B* materials with arguably unbounded numbers of shapes and sizes of *A* molecules diffusing using into equally complex solvent molecules of *B* makes measurement of *D* for every distinct combination of the two materials a distinct result worth reporting.As is also evident from Fig.(1), still even after close to two centuries of history of diffusivity measurement (since 1833 till date), the problem is receiving considerable attention of researchers [1,3,4,6-10,12]. Increasingly sophisticated methods such as (but not limited to) Coherent Quasi Elastic Neutron Scattering (QENS), Temporal Analysis of Products (TAP), DIF Microscopy, Tracer ZLC, Exchange NMR, Raman Tracer etc. are being employed to measure this important material property.

In this scenario, a novel but much simpler method employing a laser beam as an "optical marker" suggested by Dok-Yong *et al*. [1] merits a revisit and revalidation. This method belongs to the class of "non-equilibrium methods" and "direct visual observation" category. It is simple-minded, accessible to students at departmental laboratory level and yet has a general applicability to any pair of transparent solute and solvent combination in liquid state at room temperature. It uses a "radial laser beam" as an optical marker to pin-point the region of diffusion and to measure the change in optical property (refractive index) in that region as a result of the ongoing diffusion process. In their pilot study of 2017, Dok-Yong et al applied this method to measure the diffusivity of salt solution into water. However, there have not been any reports of this method having been applied to other more complex pairs of materials.As noted by Price et al [12], measurement of diffusivity of sugars has critical importance in areas ranging from Food Processing, Pharmaceutics, Cryopreservation of Proteins to Atmospheric Sciences. They employed the Raman Tracer method to measure the diffusivity of sucrose at high activity level of sucrose.

In this background, we have used the radial laser beam method of direct observation of the diffusion boundary to measure the bulk diffusivity of aqueous sucrose solution in distilled water at various concentrations. It can also be viewed as a more detailed pilot study on the applicability of this procedure. In the remainder of this article, we may interchangeably refer to the aqueous Sucrose solution and the distilled water as the minor component (or *A*) and the major component (or as *B*) respectively. In the section experimental design, we present a brief summary of the design of the ex-periment along with the theoretical framework that forms the back ground of this method. The description of the experimental setup and the procedure are provided in the next section. Followed by the results of the experimental procedure and concluding remarks also given.

THE EXPERIMENTAL DESIGN

A Schematic Representation of the Experiment

With a view to helping illustrate the theoretical framework to be developed in this section and in order to introduce the nomenclature to be used, we rst reproduce the schematic diagram of the experimental set up (as presented by Dok-Yong et al [1] in Fig. (2): The Figure 2(a) depicts the laser beam (deep dark line emerging from the semi-conductor laser) being incident on a glass rod xed at an angle with the horizontal (typically equal to 45^0) and, as a consequence, producing the so-called "radial laser beam" also inclined at angle with the horizontal as seen in Fig 2(b). In the ex-perimental procedure, rst, the cuvette is half- lled with distilled water. Then the prepared sucrose solution with desired concentration is injected slowly into the cuvette above the level of distilled water. The solution then begins to di use into the water. This radial laser beam, if and when incident on the cuvette with half-filled distilled water before the injection of the sucrose solution, traverses undisturbed to the screen xed a distance L_1 from the cuvette and is seen as the red slanted straight line as represented in Fig(2)(b). However, upon injection of the sucrose solution above the layer of distilled water and with the diffusion process setting in, a tilted bell-shaped pro le of the laser beams (as seen in Fig. (2)(c) appears on the screen. This pro le occurs due to the di erence of refractive index of the solution and distilled water across the diffusion boundary. The maximum depth of the profile *H* is due to the maximum gradient of the refractive index in the vertical (x-) direction at the point of

intersection of the laser beam and the diffusion boundary (x = 0). As the diffusion proceeds, this maximum of the gradient of refractive index decreases with time, with decrease in the concentration gradient across the two solutions, re-sulting in a gradual decrease of the maximum depth *H*. The rate of decrease of *H* as a function of time interval *t* can be measured by recording the depth of the profile on the screen. In the theoretical framework presented below, we use these quantities to obtain an expression for the diffusivity *D*.

THE THEORETICAL FRAMEWORK

The Diffusivity and Refractive Index relationship

The diffusion process in one dimension (say, along the vertical x-axis in our experi-ment) is given by Fick's second law

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2} \qquad (1)$$

In eq (1), $C(x,t)$ is the mass concentration at any position x at any time t inside a sample volume which may contain, as per the experimental design, either the sucrose solution or distilled water or a mixture of the two (as a consequence of diffusion) and D is the bulk diffusion coefficient of solution. It may be noted that the relationship between the concentration $C(x, t)$ and refractive index of a solution n(x; t) can be characterized as a linear relationship with a constant slope m and intercept n_0:,

$$n(x,t) = mC(x,t) + n_0. \qquad (2)$$

Thus the Fick's Second Law of eq.(1) can be recast in terms of n:

$$\frac{\partial n(x,t)}{\partial t} = D\frac{\partial^2 n(x,t)}{\partial x^2} \qquad (3)$$

The general solution of the Diffusion Equation (eq.(3) for our case can be written as

$$\frac{\partial n(x,t)}{\partial x} = \frac{n_2 - n_1}{2\sqrt{\pi Dt}} exp[-\frac{x^2}{4Dt}] \qquad (4)$$

where n_1 and n_2 represent the refractive indices of distilled water and that of the sucrose solution at a given concentration respectively. The equation (4) represents the gradient of refractive index near the diffusion boundary. Let us note that if we imagine that the solutions *A* and *B* are in contact with each other along the diffusion boundary perpendicular to the x-axis, with the maximum of the gradient being at x=0, then Eq. (4) provides, at x=0,

$$\{\frac{\partial n(0,t)}{\partial x}\}_{max} = \frac{n_2 - n_1}{2\sqrt{\pi Dt}}. \qquad (5)$$

From the Eqn.(5), an expression for the diffusion coefficient *D* can be readily obtained:

$$D = \frac{(n_2 - n_1)^2}{4\pi t\{\frac{\partial n(0,t)}{\partial x}\}^2_{max}} \qquad (6)$$

Therefore, if the maximum value of refractive index gradient is measured, the diffusion coefficient can be determined.

Determination of $\left\{\frac{\partial(n,t)}{\partial x}\right\}^2_{max}$:

The maximum value of the gradient of refractive index can be determined through the measurement of the maximum deviation angle of refracted rays passing through the solution layer, or more precisely, across the diffusion boundary. Let us imagine for a moment, that the radial laser beam is incident on the cuvette along a direction parallel to the x-axis. The representative parallel rays constituting the beam will undergo deviation as they pass from air into the sucrose solution in the region x > 0 and into the distilled water in the region x < 0. This situation and the angles of deviation are depicted in the Fig. (3). An incident ray undergoes angular deviation as shown in Fig. (3a) which varies with x due to di erence of refractive index of the medium (solution or water) through which it propagates. The rays that pass in the vicinity of the diffusion boundary and propagate through the region where diffusion is under process, experience an angular deviation (x; t) with the maximum deviation being at x = 0 (as shown in Fig (3b)).

In fact, the deviation angle (x; t) of the rays that propagate in the vicinity of the diffusion boundary can be expressed as

$$\beta(x,t) = \frac{\delta(n_2 - n_1)}{2\sqrt{\pi Dt}} exp(-\frac{x^2}{4Dt}) \qquad (7)$$

where (as shown in Fig. (3b)), is the thickness of the solution (or width of the cuvette) through which the rays propagate before emerging on the other side of the cuvette before reaching the screen. As argued in detail by Dok-Yong et al [1], the maximum angular deviation occurs for the ray that passes through the point x=0. Thus we obtain the relation:

$$\gamma = \beta(0,t)_{max} = \delta \frac{n_2 - n_1}{2\sqrt{\pi Dt}} \qquad (8)$$

Now, comparing equations (5) and (8), we obtain that the maximum of refractive index gradient is given by

$$(\frac{\partial n}{\partial x})_{max} = \frac{\gamma}{\delta} \qquad (9)$$

As seen in Fig. (2)(c) the maximum depth H of the tilted bell-shaped pro le is small compared to L_1, the separation between the cuvette and the screen. Therefore, the angle of maximum deviation , subtended at the point of intersection (x=0) of the tilted radial beam and the diffusion boundary can be written as

$$\gamma = \frac{H}{L_1} \qquad (10)$$

Combining the equations (6, 9 and 10), we obtain the expression for diffusivity

D:

$$D = \frac{\delta^2(n_2 - n_1)^2}{4\pi t\gamma^2} = \frac{\delta^2(n_2 - n_1)^2 L_1^2}{4\pi t H^2}. \qquad (11)$$

A practical difficulty arises if we really work with either a vertical or a horizontal radial laser beam. In the case of a vertical beam incident parallel to the x-axis on the cuvette, the incident beam and the refracted beam get superposed on the screen, thus yielding an ambiguous reading for the angle of maximum deviation. On the other hand, if the radial beam is made coincident with the diffusion boundary, a broad di racted ray pro le with fuzzy boundary line is obtained on the screen, again rendering the measurement of maximum deviation angle impossible. A slant radial beam intersecting the diffusion boundary at one point (de ned to be the origin x=0 here), produces a clear refracted

beam pro le, albeit a slanted one, thus pinpointing as an "Optical Marker" the point on the diffusion boundary where the maximum deviation of the incident ray occurs as a consequence of maximum of the refractive index gradient (or maximum concentration gradient). One might wonder whether the value of the maximum angular deviation in this slanted pro le represents the accurate value or not. However, this ambiguity is taken care of by measuring the values of maxi-mum angular deviation using incident radial beams with angles of tilt to be and 90^0 + respectively with the horizontal and then averaging the readings for a given value of the concentration of the solution. A more accurate procedure would be to digitally store the images of the tilted pro le produced with the two angles of tilt and recorded at xed times. These digital images can then be added using appropriate image processing procedures to produce accurate bell-shaped curves where from the values of *H* can be read off .

As noted by Dok-Yong et al [1], however, this angle of maximum deviation is largely independent of the angle of tilt (as long as this angle is greater than 0 and held constant during the experiment). We have therefore, kept the angle fixed, recorded the refracted laser beam profiles and noted the values of *H* from the location of maximum *H* of the tilted bell-shaped profile itself.

If we note the depths H_1 and H_2 at times t_1 and t_2 respectively, then (eq.(11) produces the final expression used to calculate the value of *D* as:

$$D = \frac{\delta^2 (n_2 - n_1)^2 L_1^2}{4\pi(\Delta t)} \left(\frac{1}{H_2^2} - \frac{1}{H_1^2}\right), \qquad (12)$$

with ⊚t = (t_2 - t_1). It may be noted here, that all the quantities on the right hand side of this equation are directly measurable.

EXPERIMENTAL SETUP AND PROCEDURE

Experimental Setup

The setup used in conducting this experiment is shown in Fig. (4). The semicon-ductor laser used has a wavelength of 635 nm and a power output of 2 mW. A cylindrical rod of diameter 0.117cm is held xed at an angle of about 60^0 with the horizontal in front of the laser source using an appropriately grooved thermocool sheet (not visible in the picture).

As seen in the image, the cuvette is placed on a raised platform so to align its contents with the laser beam produced by the laser source. The tilted bell-shaped pro le of the refracted laser beam is obtained on the graph paper screen.

Procedure

The experiment is carried out with the following procedure:

- Sucrose solution of 30% w/w is prepared by weighing 30 g of Sucrose and by mixing it with 100 g of distilled water.
- The cuvette (of inner dimensions 4.8 cm, 4.8 cm, 2.2 cm) half lled with distilled water is placed on the raised platform.This design of the cuvette provides the value = 2.2 cm. Value of L_1 is measured along the optical bench seen in the image. The slanted radial laser beam is then turned on and aligned to produce a tilted straight line pro le on the graph paper screen.
- Then 10 ml of the 30% w/w sucrose solution is injected slowly at the top of the distilled water.
- After a few seconds, (as the bulk diffusion process sets in, a tilted bell-shaped curve as seen in the image in g.(4)) appears on the graph paper screen.

- The maximum depth of this tilted bell shaped curve and the position of its base corresponding to x = H of maximum depth are noted at fixed time intervals ⊚t (noted in Tables 2 and 3) The difference of these readings at the beginning and end of the time interval ⊚t yields the values of H_1 and H_2 respectively.
- The values of refractive index n_2 of the sucrose solution is measured following the standard procedure using a traveling microscope.
- The 30% w/w sucrose solution is then diluted to 27.5% w/w by addition of appropriate addition of distilled water. And all the above steps are repeated for this concentration of the solution.

Following the above procedure, we obtain the set of refractive indices n_2 of various concentrations of sucrose solution. These values are tabulated in Table (1). The quantities needed to calculate and obtain the values of D as needed in equation (11) and obtained using the steps itemized above are tabulated in Tables (2 and 3).

RESULTS AND DISCUSSION

The Refractive Indices of Sucrose solutions

The refractive indices of the sucrose solutions with various concentrations are mea-sured following standard procedure using traveling microscopes and are tabulated in Tab (1). It may be noted that the refractive index of distilled water (the value of n_1 in Eq.(11)) is taken to be equal to its standard value, i.e. 1.3330.

Measurements of the Refracted Laser Beam Profile and Evaluation of Diffusivity *D*

As outlined earlier (Subsection 3.2), the various physical quantities in the expression for bulk diffusivity D (as in eq.(11)) are measured and tabulated in the Table 2 and Table 3. For each value of concentration, bulk diffusivity for each set of observed H_1 and H_2 are calculated and tabulated. Finally, the average bulk diffusivity for each value of concentration (C) is presented. The average bulk diffusivity D as a function of mass concentration of su-crose is plotted in g.(5). For the sake of a broad and qualitative comparison, the mutual (bulk) diffusivity of sucrose solution as a function of the mass fraction as available in literature is also presented as a subplot.

It is to be noted that the diffusivity values at high concentrations (of 25% to 30%) as seen in Figure (5a) are of the order of 10^{-6} cm^2s^{-1} as also corroborated in the Figure (5b). We also observe the same pattern of a sudden qualitative increase in diffusivity at low concentrations. However, as the concentration drops, the method presented here hits its limit of accuracy. As can be noticed in the table 3), the values of H_1 and H_2 for concentration C = 16%, di er only in the range of 0.2-0.3 cm. A small error in measurement of these values get magni ed in the values of D. This explains the increasing trend in D at concentration C = 16%. This increase can be treated as an artefact of the procedure followed here to measure the value of maximum deviation H on a graph paper sheet. It seems obvious to the authors that a technically more sound method, perhaps by using digital cameras to record these readings of H, would produce more accurate and reliable results.

CONCLUDING REMARKS

We wish to conclude with the remarks that this procedure, developed by Dok-Yong et al [1], has stood out as an alternative method to measure the diffusivity of any pair of transparent solute-solvent combination.It is also to be noted that the role of the laser beam is only that of an efficient "Optical Marker". However, a more accurate instrumentation (such as a digital camera) to record the tilted bell-shaped curves are highly desirable for more accurate and reliable results of the measurement.

REFERENCES

[1] Ju Dok-Yong, Jo Jong-Hyon, and Kim Nam-Chol. A Measurement Method of Diffusion Coefficient of Liquid Using Radial Laser Rays Formed By Cylindrical Refractive System. url: https : / / arxiv . org / ftp / arxiv / papers / 1709 / 1709.01595.pdf.

[2] Stefano Brandani, Mohamed A Jama, and Douglas M Ruthven. \ZLC Mea-surements under non-linear conditions". In: Chemical Engineering Science 55.7 (2000), pp. 1205{1212. doi: https : / / doi . org / 10 . 1016 / S0009 - 2509(99)00411-X.

[3] Cornelia Breitkopf. \Diffusion in Porous Media- Measurement and Modelling; Lecture Series at Fritz-Haber Institute, Berlin on Modern Methods in Hetero-geneous Catalysis". In: Institut fur Energietechnik, 2011.

[4] Helge Bux et al. \Ethene/ethane separation by the MOF membrane ZIF-Molecular correlation of permeation, adsorption, diffusion". In: Journal of Membrane Science 369.1-2 (2011), pp. 284{289.

[5] Christian Chmelik et al. \Exploring the nature of surface barriers on MOF Zn(tbip) by applying IR mi croscopy in high temporal and spatial resolution". In: Microporous and Mesoporous Materials 129.3 (2010), pp. 340{344.

[6] Ryota Hae et al. \Hydrogen diffusivity in wadsleyite and water distribution in the mantle transition zone". In: Earth and Planetary Science Letters 243.1-2 (2006), pp. 141{148.

[7] M A Islam. Einstein-Smoluchowski Diffusion Equation: A Discussion". In: Physica Scripta 70.2-3 (2004), p. 120.

[8] H. Jobic. \QENS and the Bene t of Diffusion Measurements over Di erent Length Scales". In: Diffusion Fundamentals 6 (2007), pp. 52.1{52.8.

[9] Jorg Karger and Rustem Valiullin. \Mass transfer in mesoporous materials: the bene t of microscopic diffusion measurement". In: Chemical Society Reviews 42.9 (2013), pp. 4172{4197.

[10] Wenjun Li et al. \The measurement of gas diffusivity in porous materials by temporal analysis of products (TAP)". In: Catalysis Today 121.3-4 (2007), pp. 246{254.

[11] Jean Philibert. \One and a Half Century of Diffusion: Fick, Einstein, Before and Beyond". In: Diffusion Fundamentals 2 (2005), pp. 1.1{1.10.

[12] Hannah C Price, Johan Mattsson, and Bejamin J. Murray. \Sucrose diffusion in aqueous solution". In: Physical Chemistry Chemical Physics 28.18 (2016), pp. 19207{19216.

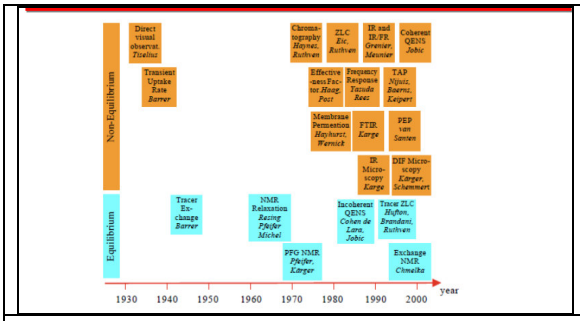


Figure 1: A graphical chronology of diffusivity measurement techniques employed over past nine decades.
(J. Kärger, University Leipzig Vasenkov & Kärger. *Magn. Res. Imag*. 23 (2005) 139.)

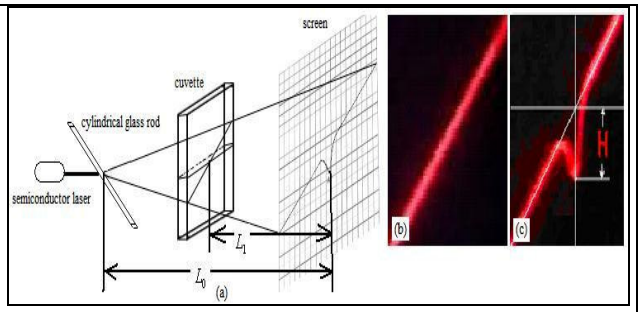


Figure 2: (a) A schematic representation of the experimental design (b) Profile of the radial laser beam (that has passed through only the half- lled distilled water in the cuvette before the injection sucrose solution above it) received on the screen; (c) Profile of the laser beam after it has passed through the diffusion boundary layer at the middle of the cuvette.

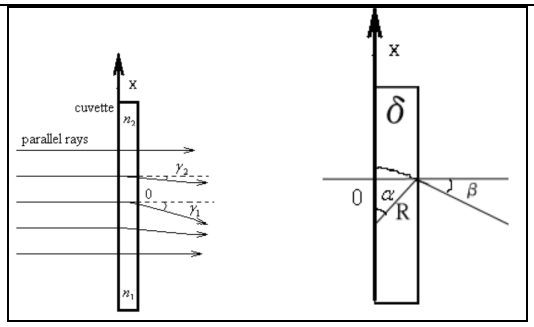


Figure 3. (a)Radial laser beam incident on the cuvette parallel to x-axis. The angles of deviation are shown upon emergence from the cuvette

Figure 3. (b) Angular Deviation (x; t) of laser rays passing close to the dif-fusion boundary in the vicinity of x=0.

Figure 3: The angular deviation of the laser beam, if incident, parallel to the vertical x-axis

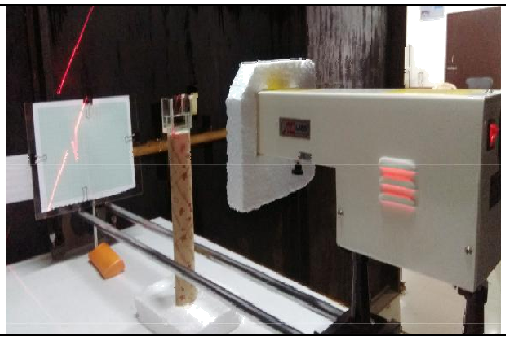
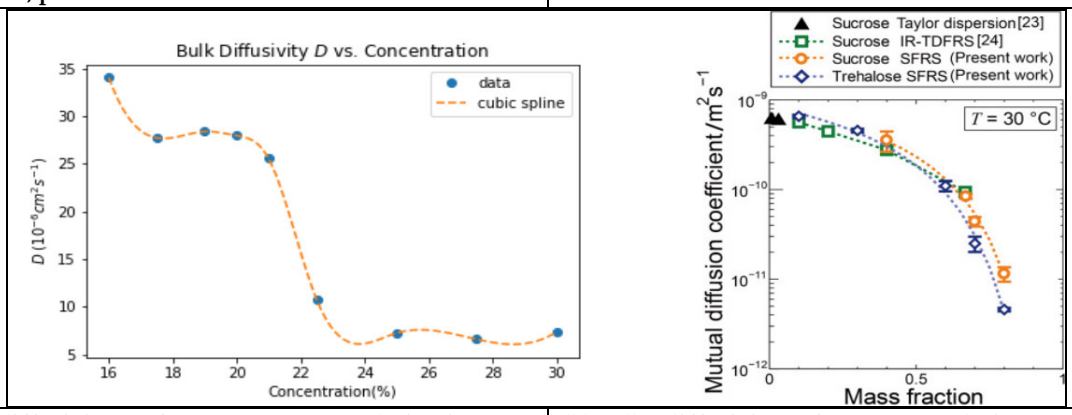


Figure 4: The setup used in conducting this experiment.



Bulk diffusivity *D* of aqueous sucrose solution in water as measured by the refracted laser beam pro le following the procedure outlined here and rst pro-posed by Dok-Yong et al [1].

(b)Bulk diffusivity of sucrose solution as a function of sucrose mass fraction as reported in lit-erature.

Figure 5: Bulk diffusivity of sucrose solution measured following the "Laser Optical Marker" method described above is plotted on the left-side figure. The figure on the right, obtained from literature is presented for a qualitative comparison

Table 1: Measured Refractive Indices for Different Concentrations of Sucrose Solution.

S.No.	Concentration (%)	Refractive Index (n_2)
1	30	1.3812
2	27.5	1.3767
3	25	1.3723
4	22.5	1.3681
5	21	1.3656
6	20	1.3639
7	19	1.3623
8	17.5	1.3598
9	16	1.3573
10	15	1.3557

Table 2: Measurements of the Tilted Refracted Bell-shaped Laser Beam Profile as seen in Fig (4) and Calculation of Diffusivity *D*.

C(%)	t (min)	L_1 (cm)	H_1 (cm)	H_2 (cm)	D	Average D
					(10 6cm2s 1)	(10 6cm2s 1))
30	15	31.6	8.0	6.4	8.705	7.341
			6.4	5.5	8.562	
			5.5	5	6.876	
			5.0	4.7	5.219	
27.5	10	56.5	11.9	11.0	4.707	6.586
			11.0	10.0	6.792	
			10.0	9.3	6.113	
			9.3	8.7	6.456	
			8.4	7.8	8.861	
25	10	35.6	8.8	7.4	6.734	7.233
			7.4	6.5	6.808	
			6.0	5.3	9.849	
			5.3	5.0	5.540	
22.5	10	43.4	9.5	7.5	9.977	10.770
			7.5	6.4	9.886	
			6.4	5.7	9.481	
			5.7	5.0	13.736	
21.0	10	49.0	5.5	4.6	23.261	25.570
			4.6	4.1	20.032	
			4.1	3.7	22.207	
			3.7	3.4	22.046	
			3.4	3.0	40.304	
					Continued..	

Table 3: Measurements of the Tilted Refracted Bell-shaped Laser Beam Profile as seen in Fig (4) and Calculation of Diffusivity *D* (Continued from previous page)

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C(%)	Δt (min)	L_1 (cm)	H_1 (cm)	H_2 (cm)	*D*	Average *D*
					(10-6 cm2s-1)	(10-6 cm2s-1)
20.0	10	29.1	5.4	4.0	14.631	27.973
			4.0	3.3	15.212	
			3.3	2.5	35.361	
			2.5	2.0	46.683	
19.0	10	50.0	4.5	3.8	27.374	28.404
			3.8	3.4	23.770	
			3.3	2.9	37.307	
			2.9	2.7	25.168	
17.5	10	45.0	4.6	3.5	32.164	27.734
			3.5	3.0	27.583	
			2.9	2.7	17.094	
			2.7	2.4	34.095	
16.0	10	50.0	2.9	2.6	27.503	34.068
			2.6	2.3	38.954	
			2.3	2.1	35.746	

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RESEARCH ARTICLE

Looking for Exoplanets in the α-Centauri System: A Spectral Analysis of its Orbital Dynamics

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ABSTRACT

Exoplanet search is a very active area of research interest of late. We propose here a method to detect existence of exoplanet by examination of the Fourier spectrum of the orbit of the host star. The orbits of the entire star planet system are generated by numerical simulation of the orbital dynamics. The method is applied to the case of α-Centauri-AB system with an assumed exoplanet in orbit around the star α-Centauri A.

Keywords: Exoplanet, Fourier spectrum, orbital dynamics

INTRODUCTION

Stars, planets and other celestial bodies and the celestial spectacles their dynamics put up for the humanity have generated great curiosity in human societies across the world, or perhaps, since the evolution of the homo sapiens . One such question of curiosity had been whether we, the humanity, are alone in this Universe. Or, there exist among the farthest reaches of this Universe other worlds where life in some form or the other exists. With the heliocentric nature of the Solar System propounded by Copernicus gaining ground, one of the earliest natural philosophers to suggest that the there indeed exist other worlds was, none other than, Giordano Bruno, who declared in the year 1584, "This space we declare to be in nite... In it are an in nity of worlds of the same kind as our own". Later on, Isaac Newton also expressed similar speculations. However, in 1995, after Mayor and Queloz announced the observation of the exoplanet 51 Peg b [1], a "Hot Jupiter" planet orbiting its star 51 Pegasi in a hitherto unknown close orbit, all these speculations about existence of "other worlds" or "exoplanets" nally were led to rest.

Two decades down the history of Astronomy and Astrophysics, we now know for sure that there are more than 4000 such planets orbiting other stars with more than a thousand candidate planets awaiting con rmation [2]. According to

current estimates, there could be billions of exoplanets orbiting the hundreds of billions of stars in the Milky Way galaxy itself. In fact, the current interest in the "Exoplanet Community" of researchers, besides the search and con rmation of new exoplanets, is also to classify the con rmed planets into various types (Rocky or Gas Giants, Hot Jupiter, Hot Neptune, Super Earth, Dwarf Planet...) and a search for planets with potential for sustaining life.The search for "Earth-like" exoplanets with potential for sustaining life has kindled a particular interest in the -Centauri star system, the set of three stars which are our nearest neighbours. There has been an intense search for "Earth-like" exoplanets in this system [3]. Both simulation type and observational close scrutiny of this star system is underway. Zhao et al [4] have analysed existing data and have found that the masses of possible Earth-like exoplanets in the habitable zones (HZ) of these stars would be in the range of $5M_{Earth}$ - $10M_{Earth}$).

In this background, we present here a numerical simulation study of the 3-body (α–Centauri *A* , α–Centauri *B*) (the closely coupled binary stars) along with a possible exoplanet. Starting with the observed orbital parameters of α–Centauri A and α–Centauri B and those of an assumed planet of mass M_P at a distance of 1 AU (the average Earth-Sun distance) from α–Centauri A , the star which it is assumed to orbit, we numerically simulate the orbital dynamics of the system. Moving over, then, to the Fourier space with the orbital coordinates α–Centauri A , we look for the spectral signatures of the presence of the planet. In the following sections we are given a brief description of the numerical procedure and the salient features of the system along with the observed and established physical parameters. Also we followed by the results and discussions have been presented with concluding remarks.

SIMULATION OF ORBITS

The Equations of Motion and their Integration

The equations of motion of a *N*-body system with masses M_i (i = 1, 2,..., *N*) located at a position $\vec{r}_i$ and moving with velocity $\vec{v}_i$ with respect to the origin of an inertial reference frame are given by:

$$\ddot{\vec{r}}_i \equiv \dot{\vec{v}}_i = -G \sum_{j=1;j\neq i}^{N} M_j \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|^3} \qquad (1)$$

where *G* is the Universal Gravitational Constant.

We use the well known Leap-Frog Algorithm, also otherwise known as the Drift-Kick-Drift method, to solve for the orbits of this system. Under this algorithm, the set of phase space vectors {$(\vec{r}_i, \vec{v}_i)$, i = 1, 2,.. *N*} are obtained by the following set of steps executed in the given order:

$$\vec{r}_i\,' = \vec{r}_i^{Present} + \vec{v}_i^{Present}(\frac{1}{2}\triangle t) \qquad (2)$$

$$\vec{v}_i^{Next} = \vec{v}_i^{Present} - G \sum_{j=1,j\neq i}^{N} M_j \frac{\vec{r}_i\,' - \vec{r}_j\,'}{|\vec{r}_i\,' - \vec{r}_j\,'|^3}\triangle t \qquad (3)$$

$$\vec{r}_i^{Next} = \vec{r}_i\,' + \vec{v}_i^{Next}(\frac{1}{2}\triangle t). \qquad (4)$$

The first step (a Drift) (eq. 2) produces an interim position vector $\vec{r}_i\,'$ using the present values of the position vector $\vec{r}_i^{Present}$ and the velocity vector $\vec{v}_i^{Present}$ over half the chosen time step, i.e. $\frac{1}{2}\Delta t$. The second step (a Kick) (eq. 3)

is produced by generating the next set of velocity vectors $\vec{v}_i^{Next}$ over a full time step Δt by using the accelerations evaluated at the interim position vectors $\vec{r}_i'$. Finally, in the last step (a Drift) (eq. 4), the next set of position vectors $\vec{r}_i^{Next}$ are evaluated with the remaining half a time step $\frac{1}{2}\Delta t$ using the set of velocity vectors at $\vec{v}_i^{Next}$ the next time step. It has been shown theoretically [5].that this algorithm conserves the phase space volume and is a lot more efficient compared to even the well-known Runge-Kutta

Runge-Kutta Algorithms when long period orbit integrations have to be carried out. In order to appreciate the e ect of an exoplanet on its star(s), we shall need to carry out the orbit integrations over a long period of time. The process begins with speci cation of the initial values $\{(\vec{r}_i(t_0), \vec{v}_i(t_0))$ i = 1, 2,.. *N*}, representing the respective "Present" set of vectors in the set of equations [2-4].

Evaluation of Initial Values

The initial values $\{(\vec{r}_i(t_0), \vec{v}_i(t_0))$ i = 1, 2,.. *N*} are the values of position and velocity vectors along the trajectory of the i^{th}-body in the Centre of Mass coordinate system at an arbitrarily chosen initial time $t = t_0$. We follow the procedure outlined by Saha and Taylor [6]. Following this prescription, we first evaluate the set of initial values of the heavier two bodies, say, *A* and *B* ($M_A > M_B$), of the system with respect to the Centre of Mass (CM) O of these two bodies. A parametric expression for the relative position vector $\vec{r}_{BA}$, that is, position of B with respect to A, can be obtained:

$$(x_{BA}, y_{BA}) = a\ (cos\ \eta - e, \sqrt{1-e^2}\ sin\ \eta) \qquad (5)$$

where *a* and *e* are, respectively, the semi-major axis and eccentricity of the orbit of *B* around the Center of Mass (CM) of the system located at one of the foci of the orbit and $\eta = \eta(t)$ is a time dependent parameter providing the solution. We need to evaluate $\eta_0(t_0)$ at the chosen initial time t_0.

We note two important orbital scale parameters for time period P_{orb} and orbital speed V_{orb} of the system:

$$P_{orb} = 2\pi\sqrt{\frac{a^3}{G(M_A+M_B)}},\quad V_{orb} = \sqrt{\frac{G(M_A+M_B)}{a}} \qquad (6)$$

Using eq. (5), we also have the magnitude of the relative position vector :

$$\vec{r}_{BA} = a(1 - e\ cos\ \eta) \qquad (7)$$

The relative angular momentum along the *z*-direction, perpendicular to the orbital plane is also obtained by using the relation

$$l_{BA,z} = x_{BA}\dot{y}_{BA} - y_{BA}\dot{x}_{BA} = V_{orb}\ a\sqrt{1-e^2}. \qquad (8)$$

Substituting in eq. (8) for the position coordinates and their time derivatives (using eq. (5)), we obtain the first order differential equation for :

$$r\frac{d\eta}{dt} = V_{orb} \tag{9}$$

whose solution with the use of eq. (7) becomes

$$t(\eta) = \frac{P_{orb}}{2\pi}(\eta - e\ sin\ \eta). \tag{10}$$

The expression for t(η) (eq.(10) is, in literature, referred to as the Kepler's Equation. It is solved numerically to obtain η_0 for a chosen value of t_0.

This value of η_0 is used in eq. (5) and the initial values of $x_{BA}(t_0)$ and $y_{BA}(t_0)$ are obtained. The initial value of the relative velocity vector is obtained using the following equations along with eqns.(5) and (10):

$$\dot{\vec{r}}_{BA}(t_0) = \frac{\frac{d\vec{r}_{BA}}{d\eta}|_{\eta_0}}{\frac{dt}{d\eta}|_{\eta_0}} \tag{11}$$

The Orbital Dynamics computer code needs input of the initial values of phase space variables ($\vec{r}_{AO}(t_0)$, $\dot{\vec{r}}_{AO}(t_0)$) and ($\vec{r}_{BO}(t_0)$, $\dot{\vec{r}}_{BO}(t_0)$) evaluated with respect to *O* (the CM) of the system. These values can be obtained by the coordinate transformation (and corresponding velocity transformation) rules to the CM frame of reference:

$$\vec{r}_{AO} = -\frac{M_B}{M_A + M_B}\vec{r}_{BA} \tag{12}$$

$$\vec{r}_{BO} = \frac{M_A}{M_A + M_B}\vec{r}_{BA} \tag{13}$$

Following a similar procedure, with respect to the CM of this 2-body system and the third body, we evaluate the initial values of all the 3-bodies with respect to the overall CM of the entire 3-body system. Using these initial values as the starting point of orbit integration in the equations (2-4), the numerical simulation code generates the orbits of the bodies.

The Fourier Spectrum of the Orbits of α–Centauri A

As the planet (with no light of its own) in the system will not be visible from the Earth, its effect on its stars has to be indirectly inferred. As the planet orbits the star A along its own orbit, its direct gravitational tug will create a small but perceptible wobble in the orbit of the star-A. As the star-A wobbles along its own orbit, it would also create a periodic tug on its partner star-B which, in turn, will also wobble in its orbit. The amplitude of this periodic wobble in the orbits of these stars would of course depend on the mass of the planet. These wobbles would be observable from the Earth. In fact, the Doppler Shift of the spectrum of the light of the stars due to these gravitational tugs from the planet(s) is used as one of the favoured methods of detection of exoplanets.We however, propose a slightly different track of analysis here. We Fourier analyze the orbits, i.e., the x- and y-coordinates of the host star (here α–Centauri A) and generate its Fourier Spectrum. The various periodicities of its motion, i.e. its orbital period around the CM of the

binary system with a smaller frequency component and the gravitational tug from the planet, a larger frequency component, and their harmonics and integral combinations of harmonics should be expressed in the Fourier Spectrum of these coordinates. Our aim is to look for the frequencies of the gravitational tug of the planet. These frequencies would be large and the corresponding energies should be small (proportional to the mass of the planet). But the presence of such peaks in the Fourier Spectrum of α–Centauri A would indicate the presence of a planet.

It may be noted that the case of α–Centauri AB plus a Planet system is just a case study, the case of the nearest neighbour of the Solar System. But in general, this procedure can be used with the observed trajectories of any star in order to look for the tell-tale signs of the existence of planets orbiting the star.

THE α–CENTAURI-AB-PLUS-PLANET SYSTEM

The α–Cen AB is a binary star system. This system along with a third star Proxima Centauri constitutes the nearest star system to the Sun, and therefore, to us, the hu-manity on the Earth. If the humanity would ever set out in hunt for an alternative planet to relocate, then an "Earth-like" planet present in the α–Centauri system would obviously be the first port of call. Therefore, the researchers' interest as stated above is obvious. As stated earlier, it is speculated that there is an exoplanet orbiting the α–Centauri A . We have applied our Orbit Integration code to study the gravitational effect of such a planet, if it does exist, on the orbits of the star α–Centauri A . At the moment, the effect of Proxima Centauri is not taken into account.

The Physical and Orbital Parameters of the α–Cen AB-plus-Planet system

The α–Cen AB System; the data provided here is taken from Wikipedia page on Alpha Centauri [7]:

- Mass of Star-A: M_A = 1:1M_S where M_S is the mass of the Sun
- Mass of star-B: M_B = 0:907M_S
- Semimajor axis of the orbit of B with respect to A ≈ Avearage Star AB distance a = 23:4 Astronomical Unit (A:U:) = 3.5×10^{12}m
- Eccentricity of the star-B orbit e = 0:5179
- Observed period of the system = 79:91Earth years = 2.520×10^{9}s
- Using equations (6), we can now calculate $P_{orb} = 2.522\times10^{9}$ s
- Also $V_{crb} - 8.722 \times 10^{3} \frac{m}{s}$
- We set t_0 = ⊚t = 10^{7}s.
- Using we obtain the numerical solution of eq. (10) and then evaluate the initial values as suggested in eqs. (5) and (11) for the relative coordinates and velocities of the stars *A* and *B*.

The Star-A Plus Planet System

- We assume four possible mass values for the planet namely, $\frac{N_P}{N_A} = 10^{-6}, 10^{-5}, 10^{-4}$ and 10^{-3}. It is worthwhile to note that these planet-star mass ratios range from the Earth-Sun to Jupiter-Sun mass ratios.
- We assume the Semi-major axis of the Planet orbit ≃ 1 AU (the Mean Sun-Earth distance = 1.496×10^{11}m $\vec{r}_{AO}(t_0)$, $\vec{r}_{AO}(t_0)$

- Initial position of the planet with respect to the Star-A: $\vec{r}_{PA}$ (t_0) = (1.496×10^{11}m; 0): (the Planet is assumed to be located on the x-axis with respect to the Star-A at the initial time t = t_0 at the measured average distance. This distance is equivalent to 1 A.U., distance at which the Earth is located with respect to the Sun.)
- Initial velocity with respect to the star-A: $\dot{\vec{r}}_{PA}(t_0)$ = (0, 3.0×10^4m/s). This is the observed average speed of the Earth around the Sun.
- The initial values of the planet with respect to the CM O of the system is then calculated by using the relations $\vec{r}_{PO}(t_0) = \vec{r}_{PA}(t_0) + \vec{r}_{AO}(t_0)$ etc.

The Initial Values

Using the above pieces the initial values in the CM-frame of the system are gener-ated. These values for the -Centauri AB -plus-Planet system with reference to its centre of mass is given below:

RESULTS AND DISCUSSION

The orbits of the 3-body system for the four assumed mass ratios of the planet with respect to α–Centauri A are plotted in Fig.1.In the plots of Fig. 1, the green line represents the orbits of the α–Centauri B , the blue spiral curves represent the orbits of the planet around its host star α–Centauri A . The orbits of α–Centauri A (red color) are seen inside the blue spiral. As the planet is bound to the gravitational field of α–Centauri A , it has a spiral orbit around its host star -Centauri A as the latter orbits around the CM of the α–Centauri AB system. The effect of the gravitational tug of the planet on the star orbits (of both A and B) are discernible only for the mass ratio 10^{-3} in the scales with which the graphs are plotted. In absolute numerical values, the e ect of the tug of the planet are seen at all mass ratios albeit in a diminishing proportion with the mass ratio from Jupiter-like mass to Earth-like mass.The "spectra" of the x-coordinates of α–Centauri A in momentum space for the four di erent mass ratios are shown in Fig 2.The plots in Fig 2, show the "power" corresponding to the various frequen-cies resulting from the two gravitational forces (one by the star α–Centauri B and the other by the planet it hosts). We know that the period of motion of the α–Centauri AB system is 79.91 years. This period corresponds to a frequency of 3.9×10^{-10} Hz. This frequency appears in the rst and most prominent peaks of all the four plots. The other 3-4 peaks are the harmonics of this frequency. The small peak at the frequency of 2×10^{-9} Hz corresponds to the frequency at which the planet tugs at the star α–Centauri A . This is the signature of the existence of the planet in orbit around α–Centauri A.

CONCLUDING REMARKS

We have presented the results of the numerical simulation of the orbital dynamics of the -Centauri AB system along with a possible exoplanet in orbit around the star α–Centauri A.The spectral analysis of the orbit of α–Centauri A suggests an alternative method for detection of existence of exoplanets in orbit around a star. This method of exoplanet detection would be worth giving a closer look. A good case in point would be to apply this method to observed orbital motion of stars.

REFERENCES

[1] M Mayor and D Queloz, "A Jupiter-mass companion to a solar-type star", Nature, vol 378, (1995) pp 355-359.
[2] "NASA Exoplanet Archive", "https://exoplanetarchive.ipac.caltech.edu/docs/ data. html"
[3] Billy Quarles, Suman Satyal, Veselin Kostov, Nathan Kaib and Nader Haghigh-ipour, "Stability Limits of Circumbinary Planets: Is There a Pile-up in the Kepler CBPs?", https://arXiv:1802.08868v1 [astro-ph.EP]

[4] Lily Zhao, Debra A. Fischer, John Brewer, Matt Giguere and Barbara Rojas-Ayala, "Planet Detectability in the Alpha Centauri System ", url = https://arXiv:1711.06320v1 [astro-ph EP]

[5] Scott Tremaine, "Geometric Methods for Orbit Integration", url = https://www.youtube com/ watch?v=2UK3Ihfr-9U&t=71s

[6] Prasenjit Saha and Paul Taylor, "The Astronomers' Magic Envelope", Oxford University Press, 2018)

[7] https://en.wikipedia.org/wiki/Alpha_Centauri.

Table 1: The Set of Initial Values for the Cen-AB-plus-Planet system with respect to its CM,O

Body	Variable (Unit)	Initial Value	
α–Cen A	$\vec{r}_{AO}(t_0)$ (m)	(-7.606×	10^{11}; -0.699×10^{11})
	$\dot{\vec{r}}_{AO}(t_0)$ (m/s)	(0.42×	10^{3}; -6.975× 10^{3})
α-Cen B	$\vec{r}_{BO}(t_0)$(m)	(9.22×	10^{11}; 0.848× 10^{11})
	$\dot{\vec{r}}_{BO}(t_0)$ (m/s)	(0.512×	10^{3}; 8.460× 10^{3})
Planet	$\vec{r}_{PO}(t_0)$(m)	(-6.109×	10^{11}; -0.699 10^{11})
	$\dot{\vec{r}}_{PO}(t_0)$(m/s)	(8:435×	10^{2}; 1:604× 10^{4})

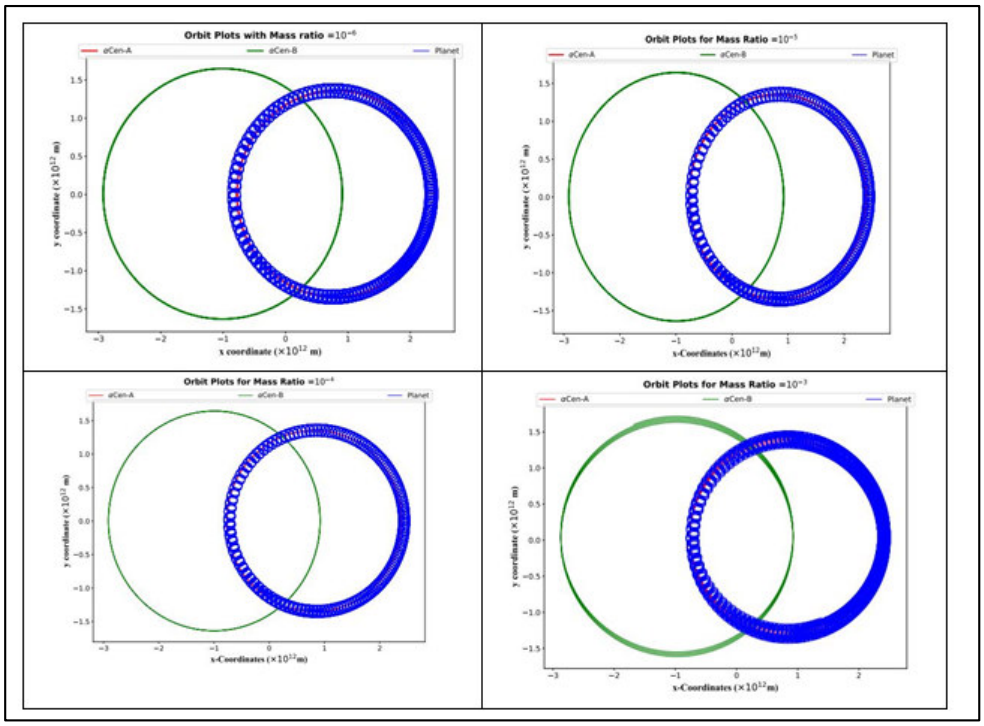

Figure 1.Set of orbits of the system for four $\frac{M_P}{M_A}$ values

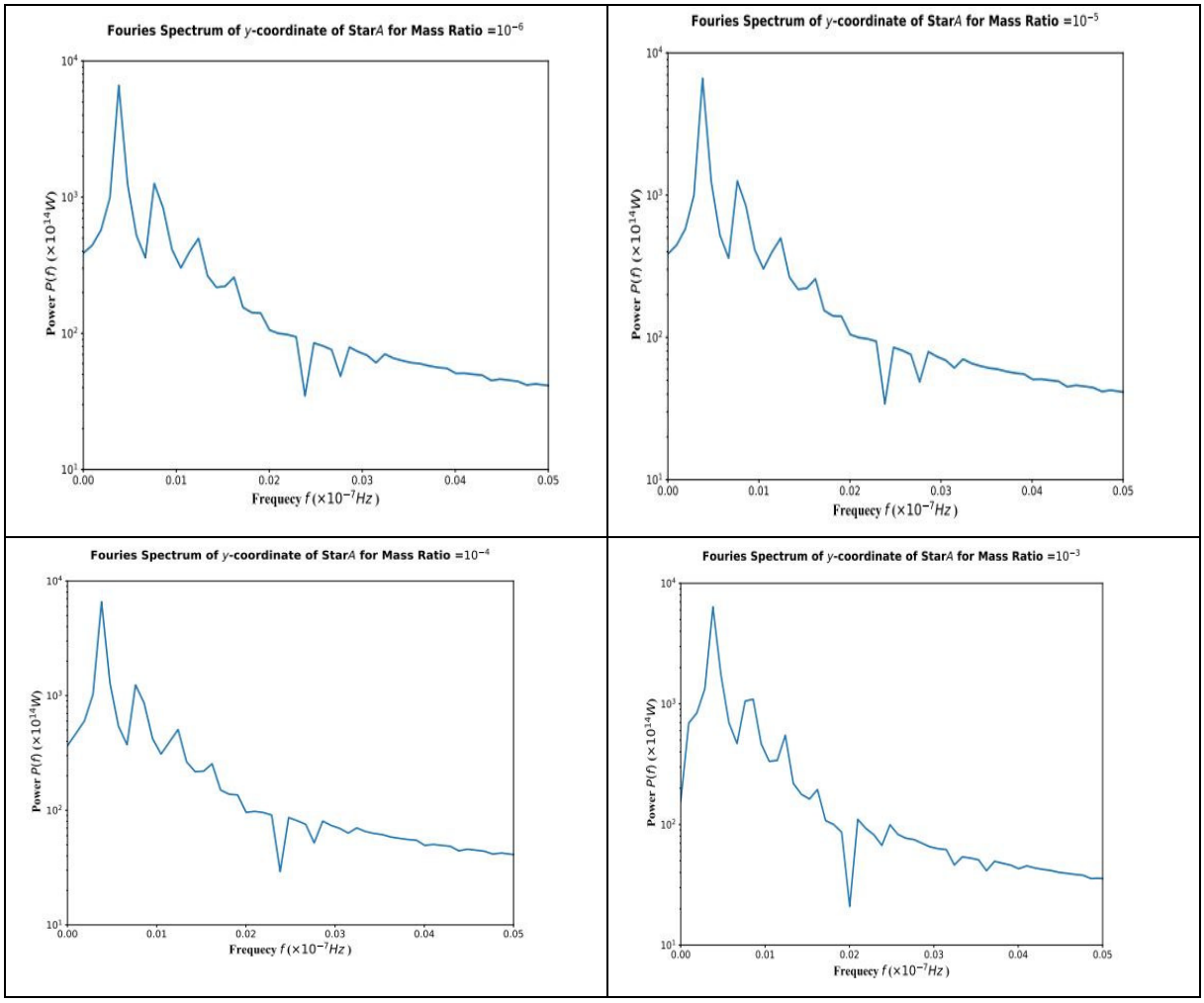

Figure 2. Set of orbits of the system for four $\frac{M_P}{M_A}$ values

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RESEARCH ARTICLE

COVID-19 Prevention by Blocking Papain like Protease 6W9C from SARS CoV-2 of Using *Aloe barbadensis* Extract: an *In silico* Analysis

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ABSTRACT

An infectious disease COVID-19 also known as "Corona virus disease 2019" which is caused by severe acute respiratory syndrome corona virus 2 (SARS-CoV-2).This global epidemic has been affecting millions of people within a short period of time. Epidemic researchers are putting lot of efforts to discover a preventive traditional vaccine. The main objective of this article is to identify the phytochemicals as ligands which has the capability to deactivate Papain like proteases from SARS CoV-2(6W9C) that help for the growth of the virus. Molecular docking of phytochemicals with the viral proteins can be studied by the Biovia Discovery studio. The interaction of molecule was determined by the energy of -CDocker and-CDocker interaction respectively. More is the negative energy means high positive scores of these two parameters indicates that Aloe-emodin can effectively inhibit the viral metabolic activity than other phytochemicals present in aloe vera It can be predicted that these molecules can interfere with the infection phase of SARS-CoV-2 virus.

Keywords: *Aloevera*, Phytochemicals, COVID-19, Biovia, SARS-CoV-2

INTRODUCTION

Globally, COVID-19 is considered as an infectious communicable serious pandemic disease. It is imparting life risk consequences for aged people in various countries. On 30th January,2020 The World Health Organization(WHO) has declared that coronavirus outbreak is a Public Health Emergency of International Concern [1,2] This epidemic were first preliminary reported at Wuhan city of China in December 2019 and gradually spread its tentacles worldwide. [3][4]. According to WHO a confirmatory case is that "if a person has undergone with laboratory confirmation of COVID-19 infection"[5]. Unfortunately till today no vaccine and preventive molecular drugs has developed to fight against this disease. [6]. Nature has been a source of many medicines in the form of chemicals, enzymes and proteins present in the plantsthrough which modern drugs have been derived [7]. The chemical substances produce by plant has some medicinal that can regulate or affect the human physiology are called as phytochemicals. These chemicals can be used as therapeutic purposes and theses phytochemicals can extract from seed, barks, leaves, fruits and

flowers etc[8]. These phytochemicals are having various medicinal properties like anti-oxidant, anti diabetic, anti-cancer and anti inflammatory. These molecules can serve as the initiators of production of pharmaceuticals which are Safe and cost effective [9]. About 25% of pharmaceutical drugs available in the market are of botanical origin and the beneficial effects are evaluated by invitro bioassay or experiments using animal models [10]. *Aloe barbadensis* belonging to family *Asphodelaceae* is known to cure many fungal, viral, bacterial and parasitic infections. It is one of the earliest known medicinal plants which is used for health benefits that has sulphur containing compounds in the form of phytochemicals.The main objective of this study to identify phytochemicals present in *Aloe barbadensis* to cure the corona virus disease COVID-19 by inhibiting its metabolism.

MATERIALS AND METHODS

Biovia software (Dassault Systems of France) having Discovery Studio tool was analysed the molecular level interaction between the phyochemicals and enzymes. This software helps in prediction of molecular interaction through machine learning . Plant produces phytochemicals as secondary metabolites to protect them from predators and plants usually fights against the micro organisms. The plant is known to contain phytochemicals likeAloe emodin, Babalocin, Anthraquinone, Glucomannan, etc Papain-like proteases from SARS CoV-2 (PDB:- 6W9C) is an enzyme that play a very crucial for the survival and multiplication of this virus.

Molecular interaction between the viral protein and phytochemicals which form a covalent bond to inhibit viral growth. Biovia discovery studio was used for analyzing the molecular interaction to identify the phytochemicals. Phytochemicals were selected from the plant and sdf file downloaded from the website. And PDB code of protein was downloaded from RCSB website. Active site as receptor cavity of this enzyme was selected as “receptor cavity” protocol found under tool "receptor-ligand interaction". For C-Docking in Biovia Discovery studio, enzyme molecule was treated as the receptor molecule and the phytochemical was treated as the ligand. Both “-CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY” were determined the strength of molecular docking. High C-Docker score considered as the efficient interaction between the phytochemicals and the viral enzyme. Therefore, high positive values predict the effect of phytochemicals on treatment of COVID-19.

RESULTS AND DISCUSSION

Active site of the 6W9C appears as light green color in fig.1. It is an insilico-based molecular docking method and optimized for accuracy. -CDOCKER energy was calculated based on the internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction signifies the energy of the nonbonded interaction that exists between the protein and the ligand. The criteria for best interaction was chosen based on a) high positive value of -CDOCKER energy and b)small difference between -CDOCKER energy and -CDOCKER interaction energy. Papainprotease and aloe emodin interaction value is represented in Table-1 and has the highest positive score of -CDOCKER energy 26.8999 kcal/mole and small value of the difference 5.6235 kcal/mole between - C DOCKER interaction energy and - C DOCKER energy. Thus, the results indicated that aloe emodin can effectively deactivate Papain protease thereby interrupting thehydrolase activity which processes the amino-terminal end of the replicase polyprotein to generate two or three replicase productsof the virus. Higher positive values for aloe emodin indicated that it was the most active ingredient against SARS-CoVvirus. Thus, the key phytochemicals aloe emodin preventing COVID-19 caused by SARS-CoV2 virus,

CONCLUSIONS

From this it is concluded that *Aloe barbadensis* has anti-viral properties against COVID-19. It is found that Aloe emodin of *Aloe barbadensis*, which can have an interaction with the viral protein Papain-like proteases significantly to prevent COVID-19. From the molecular docking analysis, It is found that aloe emodin can effectively interact with

viral protein to deactivate the viral function . othe phytochemicals do not much influence on viral protein molecule to stop their life cycle. Therefore, it can be concluded *aloe emodin* present in *Aloe barbadensis*has the medicinal values which will be help for curing COVID-19.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). Archived from the original on 31 January 2020. Retrieved 11 February 2020.
2. Mahtani, S.; Berger, M.; O'Grady, S.; Iati, M. (6 February 2020). "Hundreds of evacuees to be held on bases in California; Hong Kong and Taiwan restrict travel from mainland China". The Washington Post. Archived from the original on 7 February 2020. Retrieved 11 February 2020.
3. Naming the coronavirus disease (COVID-19) and the virus that causes it". World Health Organization (WHO). Archived from the original on 28 February 2020. Retrieved 28 February 2020.
4. Hui, D. S.; I. Azhar E.; Madani, T. A.; Ntoumi, F.; Kock, R.; Dar, O.; Ippolito, G.; Mchugh, T. D.; Memish, Z. A.; Drosten, Christian; Zumla, A.; Petersen, E. (February 2020). "The continuing 2019-nCoV epidemic threat of novel coronaviruses to global health—The latest 2019 novel coronavirus outbreak in Wuhan, China". Int J Infect Dis. 91: 264–66. doi:10.1016/j.ijid.2020.01.009. PMID 31953166.
5. Max Roser, Hannah Ritchie and Esteban Ortiz-Ospina (2020) - "Coronavirus Disease (COVID-19) – Statistics and Research". Published online at OurWorldInData.org. Retrieved from: 'https://ourworldindata.org/coronavirus' [Online Resource]
6. Sardar, Rahila, et al. "Comparative analyses of SAR-CoV2 genomes from different geographical locations and other coronavirus family genomes reveals unique features potentially consequential to host-virus interaction and pathogenesis." bioRxiv (2020).
7. Henrich J, Heine S, Norenzayan A. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X.
8. Srivastava Praveen Kumar. Achyranthes aspera: A potent immunostimulating plant for traditional medicine. International Journal of Pharmaceutical Sciences and Research. 2014;5(5):1601-1611.
9. Hussain Iqbal, Ullah Ria, Ullah Rooh, Khurram Muhammad, Ullah Naseem, Abdul Basee, Khan Farhat, Khattak Muhammad, Zahoor Muhammad, Khan, Jehangir, Khan Dr. Naeem. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
10. Wachtel-Galor S, Benzie IFF. Herbal Medicine: An introduction to its history, usage, regulation, current trends, and research needs. In: Benzie IFF, WachtelGalor S, editors. Herbal Medicine: Biomolecular and Clinical Aspects. 2nd Edition. Boca Raton (FL): CRC Press/Taylor & Francis. 2011;Chapter 1.
11. Available:https://www.ncbi.nlm.nih.gov/boo ks/NBK92773/
12. "Naming the coronavirus disease (COVID-19) and the virus that causes it". World Health Organization (WHO). Archived from the original on 28 February 2020. Retrieved 28 February 2020.
13. Hu, Ben et al. "Bat origin of human coronaviruses." Virology journal vol. 12 221. 22 Dec. 2015, doi:10.1186/s12985-015-0422-1
14. Lu, Roujian, et al. "Genomic characterisation and epidemiology of 2019 novel coronavirus: implications for virus origins and receptor binding." The Lancet 395.10224 (2020): 565-574.
15. "Coronavirus Disease 2019 (COVID-19) Symptoms". Centers for Disease Control and Prevention. United States. 10 February 2020. Archived from the original on 30 January 2020.
16. Chen, N.; Zhou, M.; Dong, X.; Qu, J.; Gong, F.; Han, Y.; Qiu, Y.; Wang, J.; Liu, Y.; Wei, Y.; Xia, J.; Yu, T.; Zhang, X.; Zhang, L. (February 2020). "Epidemiological and clinical characteristics of 99 cases of 2019 novel coronavirus pneumonia in Wuhan, China: a descriptive study". Lancet. 395 (10223): 507–513. doi:10.1016/S0140-6736(20)30211-7. PMID 32007143.

17. Gulsen Goncagul and Erol Ayaz. (2009).Uluda University, Yeni ehir brahim Orhan Vocational School, Yeni ehir/Bursa, Turkey. Antimicrobial Effect of Garlic (Aloe barbadensis). NCBI Resources. 92-93

Table 1. C-Docker results of phytochemicals of *Aloe barbadensis*with Papain protease

SL NO	Phytochemicals	- C Docker energy	- C Docker interaction energy	Difference between - C Docker interaction energy and - C Docker energy	Remark
1	Aloe emodin	26.8999	32.5234	5.6235	Aloe emodin
2	Anthraquinone	15.6616	21.1651	5.5035	Anthraquinone
3	Glucomannan	-163.892	44.468	208.36	Glucomannan
4	Babalocin	Failed	Failed	Failed	Babalocin

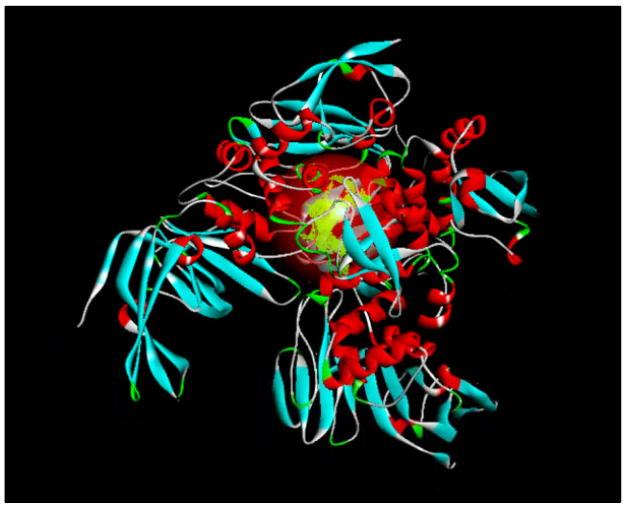

Figure 1. Active site of 6W9C

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RESEARCH ARTICLE

COVID-19 Prevention by Blocking Protease 6Y2E from SARS CoV-2 of using Aloe *barbadensis* Extract: an *In silico* Analysis

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Globally, COVID-19 is considered as an infectious communicable serious pandemic disease . It is imparting life risk consequences for aged people in various countries. On 30th January,2020 The World Health Organization(WHO) has declared that corona virus outbreak is a Public Health Emergency of International Concern [1,2] This epidemic were first preliminary reported at Wuhan city of China in December 2019 and gradually spread its tentacles worldwide. [3][4]. According to WHO a confirmatory case is that "if a person has undergone with laboratory confirmation of COVID-19 infection"[5]. Unfortunately till today no vaccine and preventive molecular drugs has developed to fight against this disease .[6]

Nature has been a source of many medicines in the form of chemicals, enzymes and proteins present in the plants through which modern drugs have been derived [7]. The chemical substances produce by plant has some medicinal that can regulate or affect the human physiology are called as phytochemicals. These chemicals can be used as therapeutic purposes and theses phytochemicals can extract from seed, barks, leaves, fruits and flowers etc. 8] . These phytochemicals are have various medicinal properties like anti-oxidant, anti diabetic, anti-cancer and anti inflammatory. These molecules can serve as the initiators of production of pharmaceuticals which are Safe and cost effective [9]. About 25% of pharmaceutical drugs available in the market are of botanical origin and the beneficial effects are evaluated by *invitro* bioassay or experiments using animal models [10]

Aloe barbadensis belonging to family *Asphodelaceae* is known to cure much fungal, viral, bacterial and parasitic infection. It is one of the earliest known medicinal plant which is used for health benefits that has sulphur containing compounds in the form of phytochemicals. The main objective of this study to identify phytochemicals present in *Aloe barbadensis* to cure the corona virus disease COVID-19 by inhibiting its metabolism.

MATERIALS AND METHODS

Biovia software (Dassault Systems of France) having Discovery Studio tool was analysed the molecular level interaction between the phyochemicals and enzymes. This software helps in prediction of molecular interaction through machine learning Plant produces phytochemicals as secondary metabolites to protect them from predators and plants usually fights against the micro organisms.Apo-like proteases from SARS CoV-2 (PDB:- 6Y2E) is a Hydrolase enzyme that play a very crucial for the survival and multiplication of this virus.

Molecular interaction between the viral protein and phytochemicals which form a covalent bond to inhibit viral growth.Biovia discovery studio was used for analyzing the molecular interaction to identify the phytochemicals. Phytochemicals were selected from the plant and sdf file downloaded from the website. And PDB code of protein was downloaded from RCSB website. Active site as receptor cavity of this enzyme was selected as “receptor cavity” protocol found under tool "receptor-ligand interaction". For C-Docking in Biovia Discovery studio, enzyme molecule was treated as the receptor molecule and the phytochemical was treated as the ligand. Both “-CDOCKER_ENERGY” and “-CDOCKER_INTERACTION_ENERGY” were determined the strength of molecular docking. High C-Docker score considered as the efficient interaction between the phytochemicals and the viral enzyme. Therefore, high positive values predict the effect of phytochemicals on treatment of COVID-19.

RESULTS AND DISCUSSION

Active site of the 6M03 appears as light green color in fig.1. It is an insilico-based molecular docking method and optimized for accuracy. -CDOCKER energy was calculated based on the internal ligand strain energy and receptor-ligand interaction energy. -CDOCKER interaction signifies the energy of the nonbonded interaction that exists between the protein and the ligand. The criteria for best interaction was chosen based on a) high positive value of -CDOCKER energy and b)small difference between -CDOCKER energy and -CDOCKER interaction energy. Apoprotease and aloe emodin interaction value is represented in Table-1 and has the highest positive score of -CDOCKER energy 18.6716 kcal/mole and small value of the difference 4.662 kcal/mole between - C DOCKER interaction energy and - C DOCKER energy. Thus, the results indicated that aloe emodin can effectively deactivate Apoprotease thereby interrupting thehydrolase activity whichprocess the amino-terminal end of the replicase polyprotein to generate two or three replicase productsof the virus . Higher positive values for aloe emodin indicated that it was the most active ingredient against SARS-CoVvirus. Thus, the key phytochemicals aloe emodin preventing COVID-19 caused by SARS-CoV2 virus

CONCLUSIONS

From this it is concluded that *Aloe barbadensis* has anti-viral properties against COVID-19. It is found that Aloe emodin of *Aloe barbadensis*, which can have an interaction with the viral protein Apo-like proteases significantly to prevent COVID-19. From the molecular docking analysis, It is found that aloe emodin can effectively interact with viral protein to deactivate the viral function of the phytochemicals do not much influence on viral protein molecule to stop their life cycle. Therefore, it can be concluded aloe emodin present in *Aloe barbadensis*has the medicinal values which will be help for curing COVID-19.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). Archived from the original on 31 January 2020. Retrieved 11 February 2020.
2. Mahtani, S.; Berger, M.; O'Grady, S.; Iati, M. (6 February 2020). "Hundreds of evacuees to be held on bases in California; Hong Kong and Taiwan restrict travel from mainland China". The Washington Post. Archived from the original on 7 February 2020. Retrieved 11 February 2020.
3. Naming the coronavirus disease (COVID-19) and the virus that causes it". World Health Organization (WHO). Archived from the original on 28 February 2020. Retrieved 28 February 2020.
4. Hui, D. S.; I. Azhar E.; Madani, T. A.; Ntoumi, F.; Kock, R.; Dar, O.; Ippolito, G.; Mchugh, T. D.; Memish, Z. A.; Drosten, Christian; Zumla, A.; Petersen, E. (February 2020). "The continuing 2019-nCoV epidemic threat of novel coronaviruses to global health—The latest 2019 novel coronavirus outbreak in Wuhan, China". Int J Infect Dis. 91: 264–66. doi:10.1016/j.ijid.2020.01.009. PMID 31953166.
5. Max Roser, Hannah Ritchie and Esteban Ortiz-Ospina (2020) - "Coronavirus Disease (COVID-19) – Statistics and Research". Published online at OurWorldInData.org. Retrieved from: 'https://ourworldindata.org/coronavirus' [Online Resource]
6. Sardar, Rahila, et al. "Comparative analyses of SAR-CoV2 genomes from different geographical locations and other coronavirus family genomes reveals unique features potentially consequential to host-virus interaction and pathogenesis." bioRxiv (2020).
7. Henrich J, Heine S, Norenzayan A. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X.
8. Srivastava Praveen Kumar. Achyranthes aspera: A potent immunostimulating plant for traditional medicine. International Journal of Pharmaceutical Sciences and Research. 2014;5(5):1601-1611.
9. Hussain Iqbal, Ullah Ria, Ullah Rooh, Khurram Muhammad, Ullah Naseem, Abdul Basee, Khan Farhat, Khattak Muhammad, Zahoor Muhammad, Khan, Jehangir, Khan Dr. Naeem. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
10. Wachtel-Galor S, Benzie IFF. Herbal Medicine: An introduction to its history, usage, regulation, current trends, and research needs. In: Benzie IFF, WachtelGalor S, editors. Herbal Medicine: Biomolecular and Clinical Aspects. 2nd Edition. Boca Raton (FL): CRC Press/Taylor & Francis. 2011;Chapter 1. Available:https://www.ncbi.nlm.nih.gov/boo ks/NBK92773/
11. "Naming the coronavirus disease (COVID-19) and the virus that causes it". World Health Organization (WHO). Archived from the original on 28 February 2020. Retrieved 28 February 2020.
12. Hu, Ben et al. "Bat origin of human coronaviruses." Virology journal vol. 12 221. 22 Dec. 2015, doi:10.1186/s12985-015-0422-1
13. Lu, Roujian, et al. "Genomic characterisation and epidemiology of 2019 novel coronavirus: implications for virus origins and receptor binding." The Lancet 395.10224 (2020): 565-574.
14. "Coronavirus Disease 2019 (COVID-19) Symptoms". Centers for Disease Control and Prevention. United States. 10 February 2020. Archived from the original on 30 January 2020.

15. Chen, N.; Zhou, M.; Dong, X.; Qu, J.; Gong, F.; Han, Y.; Qiu, Y.; Wang, J.; Liu, Y.; Wei, Y.; Xia, J.; Yu, T.; Zhang, X.; Zhang, L. (February 2020). "Epidemiological and clinical characteristics of 99 cases of 2019 novel coronavirus pneumonia in Wuhan, China: a descriptive study". Lancet. 395 (10223): 507–513. doi:10.1016/S0140-6736(20)30211-7. PMID 32007143.
16. Gulsen Goncagul and Erol Ayaz. (2009).Uluda University, Yeni ehir brahim Orhan Vocational School, Yeni ehir/Bursa, Turkey. Antimicrobial Effect of Garlic (Aloe barbadensis). NCBI Resources. 92-93

Table 1. C-Docker results of phytochemicals of *Aloe barbadensis* with Apoprotease

SL NO	Phytochemicals	- C Docker energy	- C Docker interaction energy	Difference between - C Docker interaction energy and - C Docker energy	Remark
1	Aloe emodin	18.6716	23.333	4.662	Maximum inhibition of viral protein
2	Babalocin	Failed	Failed	-	

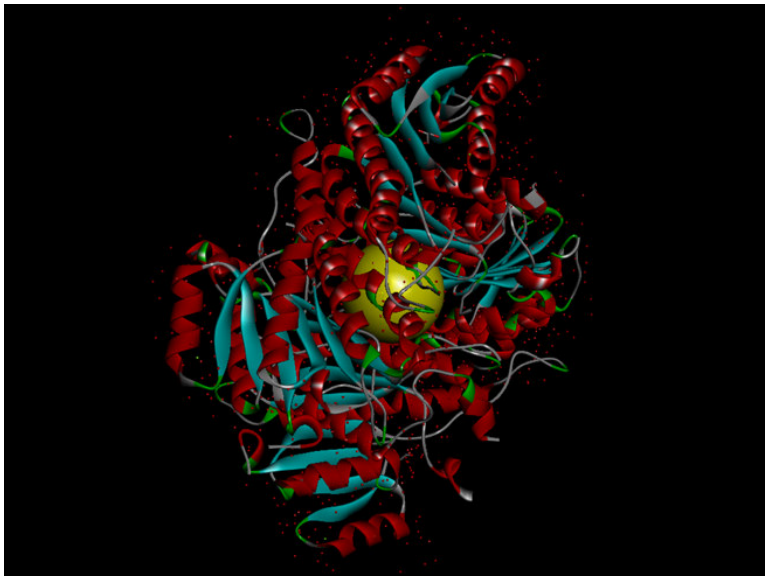

Figure 1. Active site of 6Y2E

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RESEARCH ARTICLE

COVID-19 Prevention by Blocking 6lvnE Using *Velvet bean :* an *In silico* Analysis

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ABSTRACT

An infectious disease COVID-19 also known as "Corona virus disease 2019" which is caused by severe acute respiratory syndrome corona virus 2 (SARS-CoV-2).This global epidemic has been affecting millions of people within a short period of time. Epidemic researchers are putting lot of efforts to discover a preventive traditional vaccine. As there is no specific medicines discovered to fight against the disease, researchers are working seriously to develop drugs or vaccine against COVID-19. The main aim of this study to identify the phytochemicals extracts from the plant *Velvet bean* which can deactivate 6lvn of SARS COVID-19. This deactivation can help to fight against COVID-19. The molecular C-docking of phytochemicals of *Velvet bean* were analysed by using Biovia Discovery Studio. According to the "–C Docker energy and –C Docker interaction energy" the strength of interaction was determined. For both the parameters, high positive values were considered from phytochemicasl like Dopamine. These phytochemicals deviate the enzymatic process significantly and interfere with the infection of that virus to a human cell by interrupting the life cycle of COVID-19.

Keywords: COVID-19, Biovia, *Velvet bean* ,NSP3.

INTRODUCTION

A novel corona virus (nCoV-2019) emerge as contagious disease for human on the month of December,2019 Wuhan province of China[1] and cause severe acute respiratory syndrome (SARS). On 30th January,2020 World Health Organisation has issued public health emergency of international concern under International Health regulations [2]. Situation is getting worse with this viral infection and the mortality graph approaches to upward. Therefore, the actual number is much higher than reported one and it is because of the lack of huge testing facility [3]. Shockingly, there has been no recognizable forward drive in the administration of this sickness to date and the patient is given a treatment dependent on his noticeable and diagnosable side effects [4]. Even though a few endeavors have been made in the innovative work of the diagnostics, therapeutics and immunizations for this novel corona virus, there

exists no vaccines, so far which has been demonstrated unequivocally to be viable in treating human maladies because of a tiny virus. Various traditional drugs like chloroquine, hydroxyl-chloroquine, remdesivir have effect on treatment of COVID. The less effective of these drugs motivated to examine the restraint of COVID-19 protease by Indian herbal plants [5]. Actually the therapeutic values of the herb are due to the one or more chemical compounds that participated in certain regulatory function in physiology of human. These chemicals are known as phyto-chemicals. Generally seeds, fruits, flowers, leaves, barks, flowers, roots and fruits are the main source for these medicinal values. Plant extracts of some plants have their specific function towards anti-oxidation, anti-inflammatory, anticancer and anti-diabetes etc.[6]. From ancient period plants have been used as a source of novel chemical substances which serve as a new material for the pharmaceutical industry. The leaves of bean have the following phytochemicals like alkaloids,tannins,saponin and phenolic compounds.The main objective of this article to identify the phytochemicals of *Velvet bean* responsible for inhibiting COVID-19 6MO3) by inhibiting the viral transcription and replication.

MATERIALS AND METHODS

The entire insilico analysis was done by the help of Discovery studio of "Biovia Software((Dassault Systemes de France).Molecular level of interaction can be predicted through machine learning by using this software. Plants protect itself from its predators by its own secondary metabolites. Plants may face some threats including bacteria, viruses, fungi etc. Such phytochemicals ward off health risks when certain plants or their parts are eaten by humans. Recent studies demonstrated that *Velvet bean* contains various phytochemicals like dopamine, bufotenine, behenic acid, genistine and tannic etc.. It has been reported that fabaceae have potential to fight against various diseases.This study focuses on identifying specific phytochemical which can control COVID-19[7,8]. COVID 19 can infect an individual with its various metabolic pathway. These metabolism and lifecycle are controlled by various proteins or protein like enzymes. The enzymes were identified by using Brenda database which found in COVID-19. It has been found that 6lvn is involved in multilication of virus.

By molecular docking method, it can be identified the phytochemicals which can be used as ligand and interact with the receptor of enzyme or protein of pathogen. Biovia Software's Discovery Studio modules have been used to define interaction of molecules through molecular docking. Phytochemicals of *Velvet bean* were downloaded in sdf format. The PDB code has protein database code has been identified at the RCSB website. The enzyme's active site was established through a protocol called "Define receptor binding site" found under the menu receptor-ligand interaction. The molecular docking was carried out using a C-Docker protocol by using receptor-ligand interaction. Receptor molecule was selected from the enzyme and ligands were selected from the phytochemicals. C-Docker energy and C Docker interaction energy were considered for the significant molecular CDocking. The high positive value shows the good interaction of phytochemicals with the enzyme for curing the disease.

RESULTS AND DISCUSSION

Receptor binding site of 6lvn of COVID-19 is represented as green colour in figure1. CDOCK is a simulated-annealing based molecular dynamics (MD) algorithm. It is a molecular docking process based on a grid and optimized for precision. It is an insilico based method for optimizing accuracy. Molecular Dynamic methods obtained the ligand conformations. The energy difference was calculated by-CDOCKER energy from the internal ligand strain and energy from the receptor-ligand interaction. -CDOCKER interaction refers to the energy of an unbonded interaction between the protein and the ligand. The best interaction criteria were chosen based on a) high positive value of -CDOCKER energy, and b)small difference between -CDOCKER energy and -CDOCKER energy interaction. High positive values of C-Docker energy is 11.7313 and the difference with Cdocker interaction energy 7.0.7578 are presented in table-I. From these findings it is found that Dopamine can effectively deactivate 6lvn,

thereby interrupting viral replication. Thus, the key phytochemicals Dopamine can prevent COVID-19 caused by 6lvn of virus.

CONCLUSIONS

It was reported that *Velvet bean* has shown better response to COVID-19. This study was carried out to find the phytochemical responsible for its medicinal action. From this study, it is concluded that phytochemicals like Dopamine can inhibit the lifecycle of virus causing COVID19 by using *insilico* analysis through Biovia Discover software. These molecules as ligand can have a significant interaction with 6lvn of COVID-19. It was found that Dopamine of *Velvet bean* can have strong interaction with the enzymatic molecule that inhibit the life cycle of virus. From this study it can be concluded that phyochemical Dopamine provide the medicinal importance to *Velvet bean* that can act against COVID-19 caused by 6lvn.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). Archived from the original on 31 January 2020. Retrieved 11 February 2020.
2. Mahtani, S.; Berger, M.; O'Grady, S.; Iati, M. (6 February 2020). "Hundreds of evacuees to be held on bases in California; Hong Kong and Taiwan restrict travel from mainland China". The Washington Post. Archived from the original on 7 February 2020. Retrieved 11 February 2020.
3. Sardar, Rahila, et al. "Comparative analyses of SAR-CoV2 genomes from different geographical locations and other coronavirus family genomes reveals unique features potentially consequential to host-virus interaction and pathogenesis." bioRxiv (2020).
4. Hussain Iqbal, Ullah Ria, Ullah Rooh, Khurram Muhammad, Ullah Naseem, Abdul Basee, Khan Farhat, Khattak Muhammad, Zahoor Muhammad, Khan, Jehangir, Khan Dr. Naeem. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
5. Al-Amin, M. D., Islam, M. M., Siddiqi, M. M. A., Akter, S., Ahmed, S., Haque, M. M., & Chowdhury, A. S. (2012). Neoandrographolide Isolated from Leaves of Velvet bean Nees. Dhaka University Journal of Science, 60(1), 1-3.
6. Kapata, N., Ihekweazu, C., Ntoumi, F., Raji, T., Chanda-Kapata, P., Mwaba, P., & Mfinanga, S. (2020). Is Africa prepared for tackling the COVID-19 (SARS-CoV-2) epidemic. Lessons from past outbreaks, ongoing pan-African public health efforts, and implications for the future. International Journal of Infectious Diseases, 93, 233-236.
7. Debasmita Das, Sunanya Das, Mukundjee, Pandey, Dipankar Bhattacharyay. "In silicoAnalysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacteriumtuberculosis Causing Tuberculosis", EuropeanJournal of Medicinal Plants, 2020.
8. Chang C. K.; Chen C. M.; Chiang M. H.; Hsu Y. L.; Huang T. H. Transient oligomerization of the SARS-CoV N protein—Implication for virus ribonucleoprotein packaging. PLoS One 2013, 8, e65045.

Table 1. C-Docking score of different phytochemicals with 6MO3 of COVID-19

Serial Number	Phytochemicals	- C Docker energy	- C Docker interaction Energy	Difference between - C Docker interaction and - C Docker energy
1	Dopamine	11.7316	10.9735	0.7578
2	bufotenine, behenic acid, genistine and tannic	Failed	Failed	-

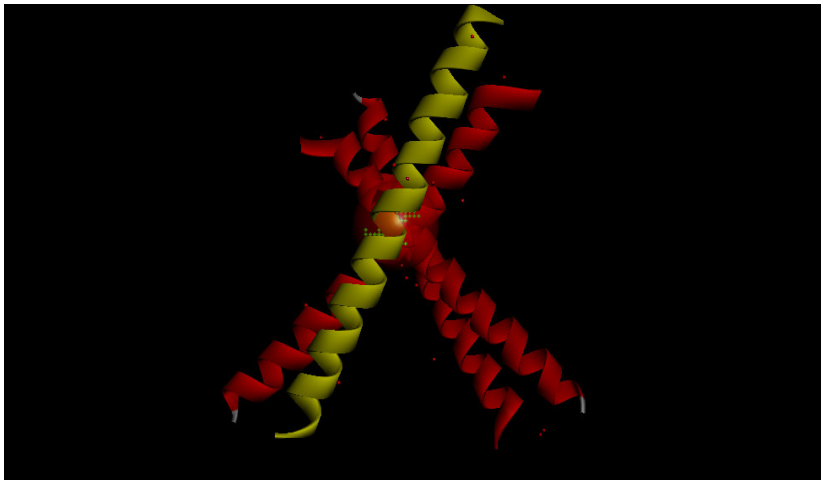

Figure 1. Binding site of 6lvn

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RESEARCH ARTICLE

COVID-19 Prevention by Blocking 6M03 Enzyme by Using Phytochemicals from *Adhatoda vasica*: an *In silico* Analysis

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ABSTRACT

Phytochemicals from *Adhatoda vasica* plant extract can cure Covid-19. It is caused by corona virus as SARS-CoV-2. Molecular interaction studied by the help of Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDocker energy and -CDocker interaction energy"suggested that quercitin can effectively deactivate the 6MO3 protease enzyme thereby inhibiting the life cycle of virus.

Keywords: Quercitin, Biovia,COVID-19 ,*Adhatoda vasica* .

INTRODUCTION

Nature is a major source of medicines[1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action[2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Adhatoda vasica* belongs to family acanthaceae. Its extract is used to cure disease like Covid-19. The objective of the study is to identify the phytochemical responsible to cure the disease. *Adhatoda vasica* has Quercitin and vasicine like phytochemicals which might be might act against Covid-19. However, there is no such study available. This objective of the study is to identify the phytochemical of *Adhatoda vasica* capable of curing corona virus disease

MATERIALS AND METHODS

"Discovery studio module of Biovia software (Dassault Systemes of France)" was used for molecular docking. Published works showed that *Adhatoda vasica* contains"Quercitin and Vasicine"etc.It was described in ancient medicinal systems capable of controlling Covid-19.

Covid-19is caused by *SARS CoV-2*.It has been found from "Brenda enzyme database" that 6MO3 protease enzyme is important in viral life cycle. Molecular docking was performed using the method described by Das et al. [4].High positive values of "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" presented a good interaction between the ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

RESULTS AND DISCUSSION

"CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm. It is a grid-based molecular docking method and optimized for accuracy. The ligand conformations were obtained by "Molecular Dynamic methods" [4]. Table 1 shows 6MO3 protease enzyme-Quercitin interaction was found to have the highest interaction.

CONCLUSIONS

Traditional medicines suggested that *Adhatoda vasica*plant has medicinal action against Covid-19 caused by COVID-19 virus. Using "Discovery studio module of Biovia software", molecular docking operation was performed. This study could explain that the presence of Quercitin is responsible for the action of *Adhatoda vasica* against Covid-19 caused by SARS CoV-2 virus.

REFERENCES

1. J Henrich, S Heine, A Norenzayan. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X
2. I. Hussain, R. Ullah, R. Ullah, M.Khurram, N. Ullah, A.Basee , F. Khan, M.Khattak, M. Zahoor, J. Khan, Dr. N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
3. P.Arulselvan, G.Karthivashan, S.Fakurazi,Journal of Chemical and Pharmaceutical Research 5 (7), 233-239, 2013
4. D. Das, S. Das, M. Pandey, D. Bhattacharyay. In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis, European Journal of Medicinal Plants, 2020.

TABLE 1. RESULTS OF CDOCKING

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Quercitin	14.2546	17.044	2.79
2	Vasicine	1.91785	16.7449	14.82705

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RESEARCH ARTICLE

COVID-19 Prevention by Blocking 6VWW Using Quercetin from *Adhatoda vasica* (Vasak) Extract: An *In silico* Analysis

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ABSTRACT

Extract from *Adhatoda vasica* has the capable to cure Covid-19.This disease is mainly caused by a virus known as SARS-CoV-2. Molecular interaction studied by the help of Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDocker energy and -CDocker interaction energy" suggested that quercetin can effectively deactivate the Uridylate-specific endoribonuclease 6VWW protease enzyme thereby inhibiting the life cycle of virus.

Keywords: quercetin , Biovia,COVID-19 ,*Adhatoda vasica*,6VWW.

INTRODUCTION

Nature is a major source of medicines [1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action [2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Adhatoda vasica* belongs to family Acanthaceae. Its extract is used to cure disease like Covid-19. The *objective of the study is to identify the phytochemical responsible to cure the disease. Adhato davasica* contains vasicine, vasicinone, peganine, quercetin, kaempferol, etc like phytochemicals which might be might act against Covid-19. However, there is no such study available. This objective of the study is to identify the phytochemical of *Adhatoda vasica* capable of curing corona virus disease

MATERIALS AND METHODS

"Discovery studio module of Biovia software (Dassault Systemes of France)" was used for molecular docking. Published works showed that *Adhatoda* avasica contains "vasicine, vasicinone, peganine, quercetin, kaempferol, etc".It was described in ancient medicinal systems capable of controlling Covid-19. Covid-19is caused by *SARS CoV-2*.It has been found from "Brenda enzyme database" that 6MO3 protease enzyme is important in viral life cycle.

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REFERENCES

1. J Henrich, S Heine, A Norenzayan. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X
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Table 1. Results of Cdocking

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Vasicine	-15.8507	30.5692	46.4199
2	Vasicinone	0.273469	15.4672	15.19373
3	Peganine	0.451414	15.0918	14.64039
4	Quercitin	25.5559	27.8617	2.3058

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RESEARCH ARTICLE

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Keywords: COVID-19, 6Y2E, Biovia, *Adhatoda vasica* ,NSP3.

INTRODUCTION

A novel corona virus (nCoV-2019) emerge as contagious disease for human on the month of December,2019 Wuhan province of China[1] and cause severe acute respiratory syndrome (SARS). On 30th January,2020 World Health Organisation has issued public health emergency of international concern under International Health regulations [2]. Situation is getting worse with this viral infection and the mortality graph approaches to upward. Therefore, the actual number is much higher than reported one and it is because of the lack of huge testing facility [3]. Shockingly, there has been no recognizable forward drive in the administration of this sickness to date and the patient is given a treatment dependent on his noticeable and diagnosable side effects [4]. Even though a few endeavours have been made in the innovative work of the diagnostics, therapeutics and immunizations for this novel corona virus, there

exists no vaccines, so far which has been demonstrated unequivocally to be viable in treating human maladies because of a tiny virus. Various traditional drugs like chloroquine, hydroxyl-chloroquine, remdesivir have effect on treatment of COVID. The less effective of these drugs motivated to examine the restraint of COVID-19 protease by Indian herbal plants [5]. Actually the therapeutic values of the herb are due to the one or more chemical compounds that participated in certain regulatory function in physiology of human. These chemicals are known as phyto-chemicals. Generally seeds, fruits, flowers, leaves, barks, flowers, roots and fruits are the main source for these medicinal values. Plant extracts of some plants have their specific function towards anti-oxidation, anti-inflammatory, anticancer and anti-diabetes etc.[6]. From ancient period plants have been used as a source of novel chemical substances which serve as a new material for the pharmaceutical industry. The leaves of vasak have the following phytochemicals like alkaloids,tannins,saponin and phenolic compounds.The main objective of this article to identify the phytochemicals of *Adhatoda vasica* responsible for inhibiting COVID-19 6Y2E by inhibiting the viral transcription and replication.

MATERIALS AND METHODS

The entire insilico analysis was done by the help of Discovery studio of "Biovia Software((Dassault Systemes de France).Molecular level of interaction can be predicted through machine learning by using this software. Plants protect itself from its predators by its own secondary metabolites. Plants may face some threats including bacteria, viruses, fungi etc. Such phytochemicals ward off health risks when certain plants or their parts are eaten by humans. Recent studies demonstrated that *Adhatoda vasica* contains Quercitin, peganine like phytocompounds.. It has been reported that Acanthacae have potential to fight against various diseases.This study focuses on identifying specific phytochemical which can control COVID-19[7,8]. COVID 19 can infect an individual with its various metabolic pathway. These metabolism and lifecycle are controlled by various proteins or protein like enzymes. The enzymes were identified by using Brenda database which found in COVID-19. It has been found that 6Y2E is involved in replication of virus.

By molecular docking method, it can be identified the phytochemicals which can be used as ligand and interact with the receptor of enzyme or protein of pathogen. Biovia Software's Discovery Studio modules have been used to define interaction of molecules through molecular docking. Phytochemicals of *Adhatoda vasica* were downloaded in sdf format. The PDB code has protein database code has been identified at the RCSB website. The enzyme's active site was established through a protocol called "Define receptor binding site" found under the menu receptor-ligand interaction. The molecular docking was carried out using a C-Docker protocol by using receptor-ligand interaction. Receptor molecule was selected from the enzyme and ligands were selected from the phytochemicals. C-Docker energy and C Docker interaction energy were considered for the significant molecular CDocking. The high positive value shows the good interaction of phytochemicals with the enzyme for curing the disease.

RESULTS AND DISCUSSION

Receptor binding site of 6Y2E of COVID-19 is represented as green colour in figure1. CDOCK is a simulated-annealing based molecular dynamics (MD) algorithm. It is a molecular docking process based on a grid and optimized for precision. It is an insilico based method for optimizing accuracy. Molecular Dynamic methods obtained the ligand conformations. The energy difference was calculated by-CDOCKER energy from the internal ligand strain and energy from the receptor-ligand interaction. -CDOCKER interaction refers to the energy of an unbonded interaction between the protein and the ligand. The best interaction criteria were chosen based on a) high positive value of -CDOCKER energy, and b)small difference between -CDOCKER energy and -CDOCKER energy interaction.

High positive values of C-Docker energy are 18.2949 and the difference with Cdocker interaction energy 4.6983 are presented in table-I.TableI also represented the difference in energy of peganine. From these findings it is found that Quercitin can effectively deactivate 6Y2E, thereby interrupting viral replication.Peganine can less effectively inhibit the viral replication as negative -CDocker energy but shows positive -CDocker interaction energy. Thus, the key phytochemicals Quercitin can prevent COVID-19 caused by 6Y2E of virus.

CONCLUSIONS

It was reported that *Adhatoda vasica* has shown better response to COVID-19. This study was carried out to find the phytochemical responsible for its medicinal action. From this study, it is concluded that phytochemicals like Quercitin can inhibit the lifecycle of virus causing COVID19 by using *insilico* analysis through Biovia Discover software. These molecules as ligand can have a significant interaction with 6Y2E of COVID-19. It was found that Quercitin of *Adhatoda vasica* can have strong interaction with the enzymatic molecule that inhibit the life cycle of virus. The following phytochemicals like, peganine were not suitable interaction with the enzyme of virus. From this study it can be concluded that these two phyochemicals Quercitin provide the medicinal importance to *Adhatoda vasica* that can act against COVID-19 caused by 6Y2E.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). Archived from the original on 31 January 2020. Retrieved 11 February 2020.
2. Mahtani, S.; Berger, M.; O'Grady, S.; Iati, M. (6 February 2020). "Hundreds of evacuees to be held on bases in California; Hong Kong and Taiwan restrict travel from mainland China". The Washington Post. Archived from the original on 7 February 2020. Retrieved 11 February 2020.
3. Sardar, Rahila, et al. "Comparative analyses of SAR-CoV2 genomes from different geographical locations and other coronavirus family genomes reveals unique features potentially consequential to host-virus interaction and pathogenesis." bioRxiv (2020).
4. Hussain Iqbal, Ullah Ria, Ullah Rooh, Khurram Muhammad, Ullah Naseem, Abdul Basee, Khan Farhat, Khattak Muhammad, Zahoor Muhammad, Khan, Jehangir, Khan Dr. Naeem. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
5. Al-Amin, M. D., Islam, M. M., Siddiqi, M. M. A., Akter, S., Ahmed, S., Haque, M. M., & Chowdhury, A. S. (2012). Neoandrographolide Isolated from Leaves of Adhatoda vasica Nees. Dhaka University Journal of Science, 60(1), 1-3.
6. Kapata, N., Ihekweazu, C., Ntoumi, F., Raji, T., Chanda-Kapata, P., Mwaba, P., & Mfinanga, S. (2020). Is Africa prepared for tackling the COVID-19 (SARS-CoV-2) epidemic. Lessons from past outbreaks, ongoing pan-African public health efforts, and implications for the future. International Journal of Infectious Diseases, 93, 233-236.
7. Debasmita Das, Sunanya Das, Mukundjee, Pandey, Dipankar Bhattacharyay. "In silicoAnalysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacteriumtuberculosis Causing Tuberculosis", EuropeanJournal of Medicinal Plants, 2020.
8. Chang C. K.; Chen C. M.; Chiang M. H.; Hsu Y. L.; Huang T. H. Transient oligomerization of the SARS-CoV N protein—Implication for virus ribonucleoprotein packaging. PLoS One 2013, 8, e65045.

Table 1. C-Docking score of different phytochemicals with 6Y2E of COVID-19

Serial Number	Phytochemicals	- C Docker energy	- C Docker interaction Energy	Difference between - C Docker interaction and - C Docker energy
1	Quercitin	21.7221	28.6056	6.8835
2	Peganine	4.43633	20.9577	16.5237

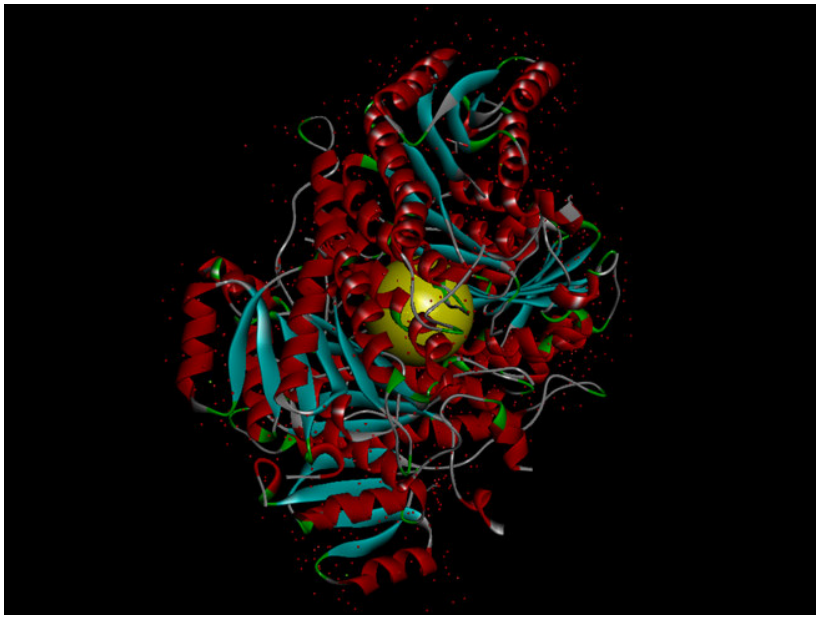

Figure 1. Binding site of 6Y2E (nucleocapsid protein N-terminal RNA binding domain)

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RESEARCH ARTICLE

COVID-19 Prevention by Blocking 6Y2E Using *Velvet bean:* An *In silico* Analysis

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ABSTRACT

An infectious disease COVID-19 also known as "Corona virus disease 2019" which is caused by severe acute respiratory syndrome corona virus 2 (SARS-CoV-2).This global epidemic has been affecting millions of people within a short period of time. Epidemic researchers are putting lot of efforts to discover a preventive traditional vaccine. As there is no specific medicines discovered to fight against the disease, researchers are working seriously to develop drugs or vaccine against COVID-19. The main aim of this study to identify the phytochemicals extracts from the plant *Velvet bean* which can deactivate 6Y2E of SARS COVID-19. This deactivation can help to fight against COVID-19. The molecular C-docking of phytochemicals of *Velvet bean* were analysed by using Biovia Discovery Studio. According to the "–C Docker energy and –C Docker interaction energy" the strength of interaction was determined. For both the parameters, high positive values were considered from phytochemicasl like bufotenine. These phytochemicals deviate the enzymatic process significantly and interfere with the infection of that virus to a human cell by interrupting the life cycle of COVID-19.

Keywords: COVID-19, Biovia, *Velvet bean* ,NSP3.

INTRODUCTION

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The entire insilico analysis was done by the help of Discovery studio of "Biovia Software((Dassault Systemes de France).Molecular level of interaction can be predicted through machine learning by using this software. Plants protect itself from its predators by its own secondary metabolites. Plants may face some threats including bacteria, viruses, fungi etc. Such phytochemicals ward off health risks when certain plants or their parts are eaten by humans. Recent studies demonstrated that *Velvet bean* contains various phytochemicals like behenic acid, genistine, and Bufotenine. It has been reported that fabaceae have potential to fight against various diseases.This study focuses on identifying specific phytochemical which can control COVID-19[7,8]. COVID 19 can infect an individual with its various metabolic pathway. These metabolism and lifecycle are controlled by various proteins or protein like enzymes. The enzymes were identified by using Brenda database which found in COVID-19. It has been found that 6Y2E is involved in multilication of virus.

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thereby interrupting viral replication. Thus, the key phytochemicals Bufotenine can prevent COVID-19 caused by 6Y2E of virus.

CONCLUSIONS

It was reported that *Velvet bean* has shown better response to COVID-19. This study was carried out to find the phytochemical responsible for its medicinal action. From this study, it is concluded that phytochemicals like Bufotenine can inhibit the lifecycle of virus causing COVID19 by using insilico analysis through Biovia Discover software. These molecules as ligand can have a significant interaction with 6Y2E of COVID-19. It was found that Bufotenine of *Velvet bean* can have strong interaction with the enzymatic molecule that inhibit the life cycle of virus. From this study it can be concluded that phyochemical Bufotenine provide the medicinal importance to *Velvet bean* that can act against COVID-19 caused by 6Y2E.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). Archived from the original on 31 January 2020. Retrieved 11 February 2020.
2. Mahtani, S.; Berger, M.; O'Grady, S.; Iati, M. (6 February 2020). "Hundreds of evacuees to be held on bases in California; Hong Kong and Taiwan restrict travel from mainland China". The Washington Post. Archived from the original on 7 February 2020. Retrieved 11 February 2020.
3. Sardar, Rahila, et al. "Comparative analyses of SAR-CoV2 genomes from different geographical locations and other coronavirus family genomes reveals unique features potentially consequential to host-virus interaction and pathogenesis." bioRxiv (2020).
4. Hussain Iqbal, Ullah Ria, Ullah Rooh, Khurram Muhammad, Ullah Naseem, Abdul Basee, Khan Farhat, Khattak Muhammad, Zahoor Muhammad, Khan, Jehangir, Khan Dr. Naeem. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
5. Al-Amin, M. D., Islam, M. M., Siddiqi, M. M. A., Akter, S., Ahmed, S., Haque, M. M., & Chowdhury, A. S. (2012). Neoandrographolide Isolated from Leaves of Velvet bean Nees. Dhaka University Journal of Science, 60(1), 1-3.
6. Kapata, N., Ihekweazu, C., Ntoumi, F., Raji, T., Chanda-Kapata, P., Mwaba, P., & Mfinanga, S. (2020). Is Africa prepared for tackling the COVID-19 (SARS-CoV-2) epidemic. Lessons from past outbreaks, ongoing pan-African public health efforts, and implications for the future. International Journal of Infectious Diseases, 93, 233-236.
7. Debasmita Das, Sunanya Das, Mukundjee, Pandey, Dipankar Bhattacharyay. "In silicoAnalysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacteriumtuberculosis Causing Tuberculosis", EuropeanJournal of Medicinal Plants, 2020.
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Table 1. C-Docking score of different phytochemicals with 6MO3 of COVID-19

Serial Number	Phytochemicals	- C Docker energy	- C Docker interaction Energy	Difference between - C Docker interaction and - C Docker energy
1	Bufotenine	11.9475	19.1818	7.2343
2	Genistine	Failed	Failed	-

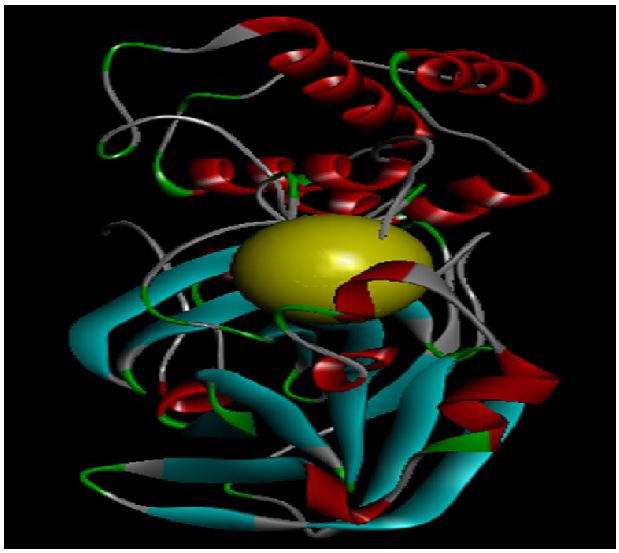

Figure 1. Binding site of 6Y2E

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RESEARCH ARTICLE

In silico Analysis of Phytochemicals by Blocking 6W6Y Enzyme of COVID-19 Using *Adhatoda vasica*

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Received: 24 Mar 2020 Revised: 25 Apr 2020 Accepted: 26 May 2020

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ABSTRACT

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REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). Archived from the original on 31 January 2020. Retrieved 11 February 2020.
2. Mahtani, S.; Berger, M.; O'Grady, S.; Iati, M. (6 February 2020). "Hundreds of evacuees to be held on bases in California; Hong Kong and Taiwan restrict travel from mainland China". The Washington Post. Archived from the original on 7 February 2020. Retrieved 11 February 2020.
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5. Al-Amin, M. D., Islam, M. M., Siddiqi, M. M. A., Akter, S., Ahmed, S., Haque, M. M., & Chowdhury, A. S. (2012). Neoandrographolide Isolated from Leaves of Adhatoda vasica Nees. Dhaka University Journal of Science, 60(1), 1-3.
6. Kapata, N., Ihekweazu, C., Ntoumi, F., Raji, T., Chanda-Kapata, P., Mwaba, P., & Mfinanga, S. (2020). Is Africa prepared for tackling the COVID-19 (SARS-CoV-2) epidemic. Lessons from past outbreaks, ongoing pan-African public health efforts, and implications for the future. International Journal of Infectious Diseases, 93, 233-236.
7. Debasmita Das, Sunanya Das, Mukundjee, Pandey, Dipankar Bhattacharyay. "In silicoAnalysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacteriumtuberculosis Causing Tuberculosis", EuropeanJournal of Medicinal Plants, 2020.
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SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Vasicine	1.3607	16.2287	14.868
2	Vasicinone	1.27036	15.9569	14.68654
3	Quercitin	19.13	22.4011	3.2711
4	Peganine	3.10266	17.7654	14.66274
5	Kaempferol	-108.715	-25.7267	82.9883

Figure 1. Binding site of 6W6Y protein of COVID-19.

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exists no vaccines, so far which has been demonstrated unequivocally to be viable in treating human maladies because of a tiny virus. Various traditional drugs like chloroquine, hydroxyl-chloroquine, remdesivir have effect on treatment of COVID. The less effective of these drugs motivated to examine the restraint of COVID-19 protease by Indian herbal plants [5]. Actually the therapeutic values of the herb are due to the one or more chemical compounds that participated in certain regulatory function in physiology of human. These chemicals are known as phyto-chemicals. Generally seeds, fruits, flowers, leaves, barks, flowers, roots and fruits are the main source for these medicinal values. Plant extracts of some plants have their specific function towards anti-oxidation, anti-inflammatory, anticancer and anti-diabetes etc.[6]. From ancient period plants have been used as a source of novel chemical substances which serve as a new material for the pharmaceutical industry.The leaves of vasak have the following phytochemicals like alkaloids,tannins,saponin and phenolic compounds.The main objective of this article to identify the phytochemicals of *Adhatoda vasica* responsible for inhibiting COVID-19 6Y2E by inhibiting the viral transcription and replication.

MATERIALS AND METHODS

The entire insilico analysis was done by the help of Discovery studio of "Biovia Software((Dassault Systemes de France).Molecular level of interaction can be predicted through machine learning by using this software. Plants protect itself from its predators by its own secondary metabolites. Plants may face some threats including bacteria, viruses, fungi etc. Such phytochemicals ward off health risks when certain plants or their parts are eaten by humans. Recent studies demonstrated that *Adhatoda vasica* contains Vasicine, peganine like phytocompounds.. It has been reported that Acanthacae have potential to fight against various diseases.This study focuses on identifying specific phytochemical which can control COVID-19[7,8].COVID 19 can infect an individual with its various metabolic pathway. These metabolism and lifecycle are controlled by various proteins or protein like enzymes. The enzymes were identified by using Brenda database which found in COVID-19. It has been found that 6Y2E is involved in replication of virus.

By molecular docking method, it can be identified the phytochemicals which can be used as ligand and interact with the receptor of enzyme or protein of pathogen. Biovia Software's Discovery Studio modules have been used to define interaction of molecules through molecular docking. Phytochemicals of *Adhatoda vasica* were downloaded in sdf format. The PDB code has protein database code has been identified at the RCSB website. The enzyme's active site was established through a protocol called "Define receptor binding site" found under the menu receptor-ligand interaction. The molecular docking was carried out using a C-Docker protocol by using receptor-ligand interaction. Receptor molecule was selected from the enzyme and ligands were selected from the phytochemicals. C-Docker energy and C Docker interaction energy were considered for the significant molecular CDocking. The high positive value shows the good interaction of phytochemicals with the enzyme for curing the disease.

RESULTS AND DISCUSSION

Receptor binding site of 6Y2E of COVID-19 is represented as green colour in figure1. CDOCK is a simulated-annealing based molecular dynamics (MD) algorithm. It is a molecular docking process based on a grid and optimized for precision. It is an insilico based method for optimizing accuracy. Molecular Dynamic methods obtained the ligand conformations. The energy difference was calculated by-CDOCKER energy from the internal ligand strain and energy from the receptor-ligand interaction. -CDOCKER interaction refers to the energy of an unbonded interaction between the protein and the ligand. The best interaction criteria were chosen based on a) high positive value of -CDOCKER energy, and b)small difference between -CDOCKER energy and -CDOCKER energy interaction.High positive values of C-Docker energy are 8.40055 and the Cdocker interaction energy 23.0537 are presented in table-I.TableI also represented the difference in energy of peganine. From these findings it is found that Vasicine can effectively deactivate 6Y2E, thereby interrupting viral replication.Peganine can less effectively

inhibit the viral replication as negative -CDocker energy but shows positive -CDocker interaction energy. Thus, the key phytochemicals Vasicine can prevent COVID-19 caused by 6Y2E of virus.

CONCLUSIONS

It was reported that *Adhatoda vasica* has shown better response to COVID-19. This study was carried out to find the phytochemical responsible for its medicinal action. From this study, it is concluded that phytochemicals like Vasicine can inhibit the lifecycle of virus causing COVID19 by using insilico analysis through Biovia Discover software. These molecules as ligand can have a significant interaction with 6Y2E of COVID-19. It was found that Vasicine of *Adhatoda vasica* can have strong interaction with the enzymatic molecule that inhibit the life cycle of virus. The following phytochemicals like, peganine were not suitable interaction with the enzyme of virus. From this study it can be concluded that these two phyochemicals Vasicine provide the medicinal importance to *Adhatoda vasica* that can act against COVID-19 caused by 6Y2E.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). Archived from the original on 31 January 2020. Retrieved 11 February 2020.
2. Mahtani, S.; Berger, M.; O'Grady, S.; Iati, M. (6 February 2020). "Hundreds of evacuees to be held on bases in California; Hong Kong and Taiwan restrict travel from mainland China". The Washington Post. Archived from the original on 7 February 2020. Retrieved 11 February 2020.
3. Sardar, Rahila, et al. "Comparative analyses of SAR-CoV2 genomes from different geographical locations and other coronavirus family genomes reveals unique features potentially consequential to host-virus interaction and pathogenesis." bioRxiv (2020).
4. Hussain Iqbal, Ullah Ria, Ullah Rooh, Khurram Muhammad, Ullah Naseem, Abdul Basee, Khan Farhat, Khattak Muhammad, Zahoor Muhammad, Khan, Jehangir, Khan Dr. Naeem. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
5. Al-Amin, M. D., Islam, M. M., Siddiqi, M. M. A., Akter, S., Ahmed, S., Haque, M. M., & Chowdhury, A. S. (2012). Neoandrographolide Isolated from Leaves of Adhatoda vasica Nees. Dhaka University Journal of Science, 60(1), 1-3.
6. Kapata, N., Ihekweazu, C., Ntoumi, F., Raji, T., Chanda-Kapata, P., Mwaba, P., & Mfinanga, S. (2020). Is Africa prepared for tackling the COVID-19 (SARS-CoV-2) epidemic. Lessons from past outbreaks, ongoing pan-African public health efforts, and implications for the future. International Journal of Infectious Diseases, 93, 233-236.
7. Debasmita Das, Sunanya Das, Mukundjee, Pandey, Dipankar Bhattacharyay. "In silicoAnalysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacteriumtuberculosis Causing Tuberculosis", EuropeanJournal of Medicinal Plants, 2020.
8. Chang C. K.; Chen C. M.; Chiang M. H.; Hsu Y. L.; Huang T. H. Transient oligomerization of the SARS-CoV N protein—Implication for virus ribonucleoprotein packaging. PLoS One 2013, 8, e65045.

Table 1. C-Docking score of different phytochemicals with 6Y2E of COVID-19

Serial Number	Phytochemicals	- C Docker energy	- C Docker interaction Energy	Difference between - C Docker interaction and - C Docker energy
1	Vasicine	8.40055	23.0537	14.65315
2	Peganine	4.43633	20.9577	16.5237

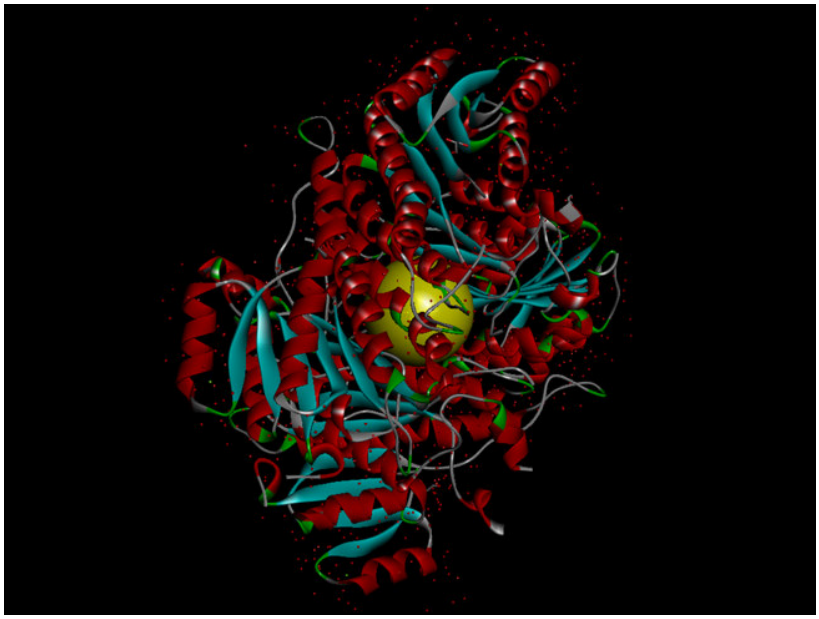

Figure 1. Binding site of 6Y2E protein

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RESEARCH ARTICLE

In silico Analysis of Phytochemicals by Blocking Papain like Protease 6W9C Enzyme of Covid-19 Using *Adhatoda vasica*

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ABSTRACT

An infectious disease COVID-19 also known as "Corona virus disease 2019" which is caused by severe acute respiratory syndrome corona virus 2 (SARS-CoV-2).This global epidemic has been affecting millions of people within a short period of time. Epidemic researchers are putting lot of efforts to discover a preventive traditional vaccine. As there is no specific medicines discovered to fight against the disease, researchers are working seriously to develop drugs or vaccine against COVID-19. The main aim of this study to identify the phytochemicals extracts from the plant *Adhatoda vasica* which can deactivate 6W9C of SARS COVID-19. This deactivation can help to fight against COVID-19. The molecular C-docking of phytochemicals of *Adhatoda vasica* (Vasak) were analysed by using Biovia Discovery Studio. According to the "–C Docker energy and –C Docker interaction energy" the strength of interaction was determined. For both the parameters, high positive values were considered from phytochemicasl like Quercitin. These phytochemicals deviate the enzymatic process significantly and interfere with the infection of that virus to a human cell by interrupting the life cycle of COVID-19.

Keywords: COVID-19, 6W9C, Biovia, *Adhatoda vasica*, Quercitin.

INTRODUCTION

A novel corona virus (nCoV-2019) emerge as contagious disease for human on the month of December,2019 Wuhan province of China[1] and cause severe acute respiratory syndrome (SARS). On 30th January,2020 World Health Organisation has issued public health emergency of international concern under International Health regulations [2]. Situation is getting worse with this viral infection and the mortality graph approaches to upward.Therefore, the actual number is much higher than reported one and it is because of the lack of huge testing facility [3]. Shockingly, there has been no recognizable forward drive in the administration of this sickness to date and the patient is given a treatment dependent on his noticeable and diagnosable side effects [4]. Even though a few endeavors have been made in the innovative work of the diagnostics, therapeutics and immunizations for this novel corona virus, there

exists no vaccines, so far which has been demonstrated unequivocally to be viable in treating human maladies because of a tiny virus. Various traditional drugs like chloroquine, hydroxyl-chloroquine, remdesivir have effect on treatment of COVID. The less effective of these drugs motivated to examine the restraint of COVID-19 protease by Indian herbal plants [5]. Actually the therapeutic values of the herb are due to the one or more chemical compounds that participated in certain regulatory function in physiology of human. These chemicals are known as phyto-chemicals. Generally seeds, fruits, flowers, leaves, barks, flowers, roots and fruits are the main source for these medicinal values. Plant extracts of some plants have their specific function towards anti-oxidation, anti-inflammatory, anticancer and anti-diabetes etc.[6]. From ancient period plants have been used as a source of novel chemical substances which serve as a new material for the pharmaceutical industry.The leaves of vasak have the following phytochemicals like alkaloids,tannins,saponin and phenolic compounds.The main objective of this article to identify the phytochemicals of *Adhatoda vasica* responsible for inhibiting COVID-19 6W9C by inhibiting the viral transcription and replication.

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The entire insilico analysis was done by the help of Discovery studio of "Biovia Software((Dassault Systemes de France).Molecular level of interaction can be predicted through machine learning by using this software. Plants protect itself from its predators by its own secondary metabolites. Plants may face some threats including bacteria, viruses, fungi etc. Such phytochemicals ward off health risks when certain plants or their parts are eaten by humans. Recent studies demonstrated that *Adhatoda vasica* contains contain Vasicine, Vasicinone, Quercitin, Peganine, and Kaempferol like phytochemicals. It has been reported that Acanthacae have potential to fight against various diseases.This study focuses on identifying specific phytochemical which can control COVID-19[7,8]. COVID 19 can infect an individual with its various metabolic pathways. These metabolism and lifecycle are controlled by various proteins or protein like enzymes. The enzymes were identified by using Brenda database which found in COVID-19. It has been found that 6W9C is involved in multiplication of virus.

By molecular docking method, it can be identified the phytochemicals which can be used as ligand and interact with the receptor of enzyme or protein of pathogen. Biovia Software's Discovery Studio modules have been used to define interaction of molecules through molecular docking. Phytochemicals of *Adhatoda vasica* were downloaded in sdf format. The PDB code has protein database code has been identified at the RCSB website. The enzyme's active site was established through a protocol called "Define receptor binding site" found under the menu receptor-ligand interaction. The molecular docking was carried out using a C-Docker protocol by using receptor-ligand interaction. Receptor molecule was selected from the enzyme and ligands were selected from the phytochemicals. C-Docker energy and C Docker interaction energy were considered for the significant molecular CDocking. The high positive value shows the good interaction of phytochemicals with the enzyme for curing the disease.

RESULTS AND DISCUSSION

Receptor binding site of 6W9C of COVID-19 is represented as green colour in figure1. CDOCK is a simulated-annealing based molecular dynamics (MD) algorithm. It is a molecular docking process based on a grid and optimized for precision. It is an insilico based method for optimizing accuracy. Molecular Dynamic methods obtained the ligand conformations. The energy difference was calculated by-CDOCKER energy from the internal ligand strain and energy from the receptor-ligand interaction. -CDOCKER interaction refers to the energy of an unbonded interaction between the protein and the ligand. The best interaction criteria were chosen based on a) high positive value of -CDOCKER energy, and b)small difference between -CDOCKER energy and -CDOCKER energy interaction.

High positive values of Quercitin C-Docker energy are 26.2435 and the difference between CDocker interaction energy 3.0409 are presented in table-I. TableI also represented the difference in energy of Vasicine, Vasicinone and peganine. From these findings it is found that Quercitine can effectively deactivate 6W9C, thereby interrupting viral replication. Vasicine, Vasicinone and peganine can less effectively inhibit the viral replication as negative -CDocker energy but shows positive -CDocker interaction energy. Thus, the key phytochemicals Quercitin can prevent COVID-19 caused by 6W9C of virus.

CONCLUSIONS

It was reported that *Adhatoda vasica* has shown better response to COVID-19. This study was carried out to find the phytochemical responsible for its medicinal action. From this study, it is concluded that phytochemicals like Vasicine, Vasicinone and Quercitin can inhibit the lifecycle of virus causing COVID19 by using insilico analysis through Biovia Discover software. These molecules as ligand can have a significant interaction with 6W9C of COVID-19. It was found that Quercitin of *Adhatoda vasica* can have strong interaction with the enzymatic molecule that inhibit the life cycle of virus. The following phytochemicals like Vasicine, Vasicinone and peganine, were not suitable interaction with the enzyme of virus. From this study it can be concluded that these two phyochemicals Quercitin provide the medicinal importance to *Adhatoda vasica* that can act against COVID-19 caused by 6W9C papain like protease.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). Archived from the original on 31 January 2020. Retrieved 11 February 2020.
2. Mahtani, S.; Berger, M.; O'Grady, S.; Iati, M. (6 February 2020). "Hundreds of evacuees to be held on bases in California; Hong Kong and Taiwan restrict travel from mainland China". The Washington Post. Archived from the original on 7 February 2020. Retrieved 11 February 2020.
3. Sardar, Rahila, et al. "Comparative analyses of SAR-CoV2 genomes from different geographical locations and other coronavirus family genomes reveals unique features potentially consequential to host-virus interaction and pathogenesis." bioRxiv (2020).
4. Hussain Iqbal, Ullah Ria, Ullah Rooh, Khurram Muhammad, Ullah Naseem, Abdul Basee, Khan Farhat, Khattak Muhammad, Zahoor Muhammad, Khan, Jehangir, Khan Dr. Naeem. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
5. Al-Amin, M. D., Islam, M. M., Siddiqi, M. M. A., Akter, S., Ahmed, S., Haque, M. M., & Chowdhury, A. S. (2012). Neoandrographolide Isolated from Leaves of Adhatoda vasica Nees. Dhaka University Journal of Science, 60(1), 1-3.
6. Kapata, N., Ihekweazu, C., Ntoumi, F., Raji, T., Chanda-Kapata, P., Mwaba, P., & Mfinanga, S. (2020). Is Africa prepared for tackling the COVID-19 (SARS-CoV-2) epidemic. Lessons from past outbreaks, ongoing pan-African public health efforts, and implications for the future. International Journal of Infectious Diseases, 93, 233-236.
7. Debasmita Das, Sunanya Das, Mukundjee, Pandey, Dipankar Bhattacharyay. "In silicoAnalysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacteriumtuberculosis Causing Tuberculosis", EuropeanJournal of Medicinal Plants, 2020.
8. Chang C. K.; Chen C. M.; Chiang M. H.; Hsu Y. L.; Huang T. H. Transient oligomerization of the SARS-CoV N protein—Implication for virus ribonucleoprotein packaging. PLoS One 2013, 8, e65045.

Table 1. C-Docking score of different phytochemicals with 6W9C of COVID-19

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Vasicine	-13.5794	34.8701	48.4495
2	Vasicinone	5.98834	20.8737	14.88536
3	Quercitin	26.2435	29.2844	3.0409

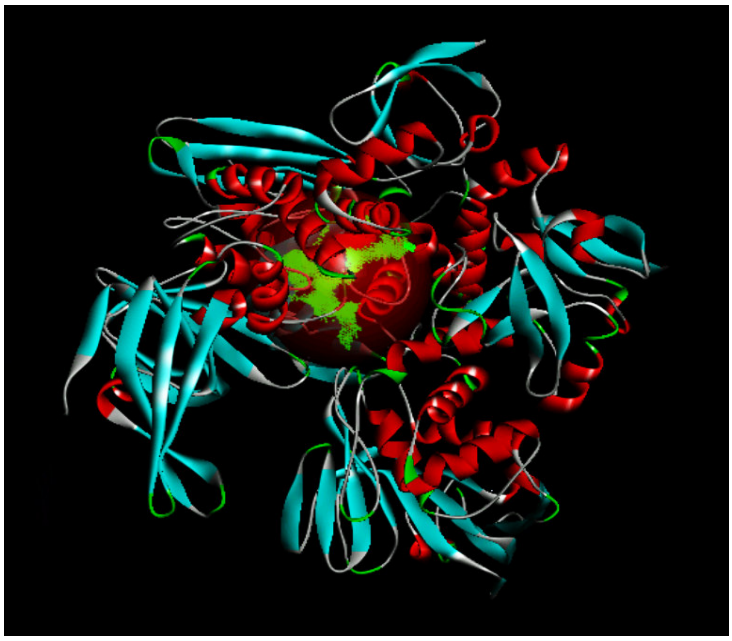

Figure 1. Binding site of 6W9C protein of COVID-19.

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RESEARCH ARTICLE

In silico Analysis of Photochemicals from *Adhatoda vasica* against 6VWW COVID-19

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ABSTRACT

Phytochemicals from *Adhatoda vasica* plant extract can cure Covid-19. It is caused by corona virus as SARS-CoV-2. Molecular interaction studied by the help of Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDocker energy and -CDocker interaction energy" suggested that Kaempferol can effectively deactivate the Uridylate-specific endoribonuclease 6VWW protease enzyme thereby inhibiting the life cycle of virus.

Keywords: Kaempferol , Biovia,COVID-19 ,*Adhatoda vasica*,6VWW.

INTRODUCTION

Nature is a major source of medicines [1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action [2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Adhatoda vasica* belongs to family Acanthaceae. Its extract is used to cure disease like Covid-19. The *objective of the study is to identify the phytochemical responsible to cure the disease. Adhato davasica* contains vasicine, vasicinone, peganine, quercetin, kaempferol, etc like phytochemicals which might be might act against Covid-19. However, there is no such study available. This objective of the study is to identify the phytochemical of *Adhatoda vasica* capable of curing corona virus disease

MATERIALS AND METHODS

"Discovery studio module of Biovia software (Dassault Systemes of France)" was used for molecular docking. Published works showed that *Adhatoda* avasica contains "vasicine, vasicinone, peganine, quercetin, kaempferol, etc".It was described in ancient medicinal systems capable of controlling Covid-19.
Covid-19is caused by *SARS CoV-2*.It has been found from "Brenda enzyme database" that 6MO3 protease enzyme is important in viral life cycle. Molecular docking was performed using the method described by Das et al. [4].High

positive values of "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" presented a good interaction between the ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

RESULTS AND DISCUSSION

"CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm. It is a grid-based molecular docking method and optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods" [4]. Table 1 shows Uridylate-specific endoribonuclease enzyme-kaempferol interaction was found to have the highest interaction.

CONCLUSIONS

Traditional medicines suggested that *Adhatoda vasica* plant has medicinal action against Covid-19 caused by COVID-19 virus. Using "Discovery studio module of Biovia software", molecular docking operation was performed. This study could explain that the presence of Kaempferol is responsible for the action of *Adhatoda vasica* against 6VWW of Covid-19 caused by SARS CoV-2 virus.

REFERENCES

1. J Henrich, S Heine, A Norenzayan. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X
2. I. Hussain, R. Ullah, R. Ullah, M.Khurram, N. Ullah, A.Basee , F. Khan, M.Khattak, M. Zahoor, J. Khan, Dr. N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
3. P.Arulselvan, G.Karthivashan, S.Fakurazi,Journal of Chemical and Pharmaceutical Research 5 (7), 233-239, 2013
4. D. Das, S. Das, M. Pandey, D. Bhattacharyay. In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis, European Journal of Medicinal Plants, 2020.

Table 1. Results of C docking

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Vasicine	-15.8507	30.5692	46.4199
2	Vasicinone	0.273469	15.4672	15.19373
3	Peganine	0.451414	15.0918	14.64039
4	Kaempferol	18.0879	22.3375	4.2496

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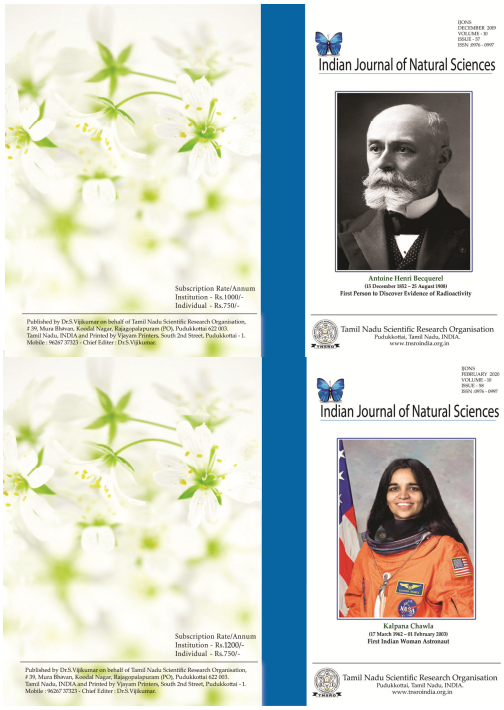

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Plant More Trees *Love Animals* *Conserve our Nature*

Conserve Our Blue Ocean…..Conserve Our Marine Resources……

World Oceans Day provides an opportunity to honor, help protect, and conserve the ocean. This year, the Day will convene under the theme, 'Innovation for a Sustainable Ocean'.

Many countries have celebrated this special day since 1992, following the United Nations Conference on Environment and Development, held in Rio de Janeiro. In 2008, the United Nations General Assembly decided that, as of 2009, 8 June would be designated by the United Nations as "World Oceans Day".Seventy per cent of our planet is covered by one huge, continuous body of seawater – the ocean. It holds 1.35 billion cubic kilometres of water. Nearly half of the ocean is more than 3 kilometres deep. The deepest known point of the ocean is in the Mariana Trench, 11 kilometres below sea level. But there may be deeper points that we have not seen, as we have only explored five per cent of the ocean to date.One of the main aims of the day is to remind people of the important role the ocean plays in our lives. Life began in the ocean. And the ocean is home to the majority of plants and animals on Earth, from single-cell organisms to the blue whale. Marine plants provide us with 70 per cent of the oxygen we breathe. The ocean controls the climate, providing heat in winter and cool air in summer. It also provides us with food and medicines as well as transport. No matter where you live on the planet, no matter how far from the sea, your life is dependent on the ocean.The most urgent problem facing the ocean at the moment is plastic pollution. Reducing one use plastic, including plastic bags and plastic bottles, has been an important theme for World Oceans Day for a number of years. Climate change and rising sea temperatures are also a huge problem. Rising sea temperatures have a direct influence on weather patterns and are seen as partly responsible for an increase in extreme weather conditions. An increase in carbon dioxide is increasing the acid levels of seawater and putting many marine organisms at risk. On World Oceans Day, wear blue, go on a march, find a beach or river clean-up near you, organise a local event, print a poster and put it in your window, or use the hashtag #worldoceansday on social media. There are so many things you can do on 8 June to join in the celebrations, to remind people about the importance of the ocean in our lives and to make a difference!

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RESEARCH ARTICLE

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ABSTRACT

Phytochemicals from *Aloe vera* plant extract can be used for the treatment of COVID-19. The causative agent for this disease is SARS CoV-2 virus. "Biovia Discovery Studio" was used to analyse the molecular docking. "High positive values of -CDocker energy and -CDocker interaction energy"suggested that Aloe-emodin can effectively deactivate Uridylate-specific endoribonuclease **(**6VWW) thereby interrupting the life cycle of the organism.

Keywords: phytochemical, Discovery studio, *Aloe vera* ,COVID-19

INTRODUCTION

Nature is a major source of medicines [1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action [2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Aloe vera* belongs to family Asphodelaceae or Lilliaceae. Aloe vera extract is used to cure disease like COVID-19. The objective of the study is to identify the phytochemical responsible to cure the disease. *Aloe vera* contains"Aloe-emodin, Cinnamic acid, Salicylic acid, Lupeol, Babalocin, Saponin"etc. These phytochemicals might act against Corona virus. However, there is no such study available. This objective of the study is to identify the phytochemical of *aloe vera* capable of curing COVID-19.

MATERIALS AND METHODS

"Discovery studio module of Biovia software (Dassault Systemes of France)" was used for molecular docking. Published works showed that *Aloe vera*contains phyto chemicals such as Aloe-emodin, Cinnamic acid, Salicylic acid, Lupeol, Babalocin, Saponin" etc.It was described in ancient medicinal systems capable of controlling COVID-19..
Corona virus disease is caused by SARS CoV-2. It has been found from "Brenda enzyme database" Uridylate-specific endoribonuclease (6VWW) is important in microbial life cycle.

Molecular docking was performed using the method described by Das et al. [4].High positive values of "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" presented a good interaction between the ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

RESULTS AND DISCUSSION

"CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm. It is a grid-based molecular docking method and optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods" [4]. Table 1 shows Uridylate-specific endoribonuclease (6VWW)- Aloe-emodin interaction was found to have the highest interaction.

CONCLUSIONS

Traditional medicines suggested that aloe vera plant has medicinal action against COVID-19 caused by SARS CoV-2. Using "Discovery studio module of Biovia software", molecular docking operation was performed. This study could explain that the presence of Aloe-emodin acid is responsible for the action of aloevera gainst COVID-19.

REFERENCES

1. J Henrich, S Heine, A Norenzayan. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X
2. I. Hussain, R. Ullah, R. Ullah, M.Khurram, N. Ullah, A.Basee , F. Khan, M.Khattak, M. Zahoor, J. Khan, Dr. N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.

Table 1. Results of C docking

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Aloe emodin	20.9121	25.1702	4.2581
2	Cinnamic acid	13.9567	18.5773	4.6206
3	Salicylic acid	12.3597	14.9839	2.6242
4	Anthraquinone	13.4088	15.4386	2.0298
5	Gluocomanan	-23.7223	54.5145	78.2368
6	Saponin	Failed	Failed	Failed

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RESEARCH ARTICLE

In silico Analysis of Phytochemicals from *Aloe vera* against 6W6Y Enzyme of COVID-19

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ABSTRACT

Phytochemicals from *Aloe vera* plant extract can treat COVID-19. It is caused by corona virus SARS CoV-2. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDocker energy and -CDocker interaction energy" suggested that Salicylic acid can effectively deactivate ADP ribose phosphatase of NSP3 (6W6Y) thereby interrupting the life cycle of the organism.

Keywords: phytochemical, Biovia, Discovery studio,*Aloe vera* ,COVID-19

INTRODUCTION

Nature is a major source of medicines [1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action [2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Aloe vera* belongs to family Asphodelaceae. Aloe vera extract is used to cure disease like COVID-19. The objective of the study is to identify the phytochemical responsible to cure the disease. *Aloe vera* contains"Cinnamic acid, Salicylic acid, Lupeol, Babalocin, Saponin"etc. These phytochemicals might act against Corona virus. However, there is no such study available. This objective of the study is to identify the phytochemical of *aloevera* capable of curing COVID-19.

MATERIALS AND METHODS

"Discovery studio module of Biovia software (Dassault Systemes of France)" was used for molecular docking Published works showed that *Aloe vera*contains phyto chemicals such as Cinnamic acid, Salicylic acid, Lupeol, Babalocin, Saponin" etc.It was described in ancient medicinal systems capable of controlling COVID-19. Corona virus disease is caused by SARS CoV-2. It has been found from "Brenda enzyme database" ADP ribose phosphatase of NSP3 (6W6Y) is important in microbial life cycle.

Molecular docking was performed using the method described by Das et al. [4].High positive values of "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" presented a good interaction between the ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

RESULTS AND DISCUSSION

"CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm. It is a grid-based molecular docking method and optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods" [4]. Table 1 shows ADP ribose phosphatase of NSP3 (6W6Y)-salicylic acid interaction was found to have the highest interaction.

CONCLUSIONS

Traditional medicines suggested that aloe vera plant has medicinal action against COVID-19 caused by SARS CoV-2. Using "Discovery studio module of Biovia software", molecular docking operation was performed. This study could explain that the presence of Salicylic acid is responsible for the action of aloevera gainst COVID-19.

REFERENCES

1. J Henrich, S Heine, A Norenzayan. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X
2. I. Hussain, R. Ullah, R. Ullah, M.Khurram, N. Ullah, A.Basee , F. Khan, M.Khattak, M. Zahoor, J. Khan, Dr. N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
3. P.Arulselvan, G.Karthivashan, S.Fakurazi,Journal of Chemical and Pharmaceutical Research 5 (7), 233-239, 2013
4. D. Das, S. Das, M. Pandey, D. Bhattacharyay. In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis, European Journal of Medicinal Plants, 2020

Table 1. Results of C Docking

SL NO	LIGAND	- C DOCKER ENERGY	- C DOCKER INTERACTION ENERGY	Difference between - C DOCKER interaction energy and - C DOCKER energy
1	Cinnamic acid	17.6225	19.6352	2.0127
2	Salicylic acid	17.6553	22.1108	4.4555
3	Lupeol	Failed	Failed	Failed
4	Babalocin	Failed	Failed	Failed
5	Saponin	Failed	Failed	Failed

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RESEARCH ARTICLE

In silico Analysis of Phytochemicals from *Filipendula ulmaria* against COVID-19

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ABSTRACT

Phytochemicals from *filipendula ulmaria* plant extract can cure COVID-19. It is caused by a virus knowns as SARS CoV-2. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDocker energy and -CDocker interaction energy"suggested that 4-hydroxycalcone can effectively deactivate 6W4B thereby interrupting the life cycle of the organism.

Keywords: phytochemical, Biovia, Discovery studio, *filipendula ulmaria*,6W4B

INTRODUCTION

Nature is a major source of medicines[1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action[2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Filipendula ulmaria* belongs to family Rosaceae. *Filipendula ulmaria* extract is used to cure disease like Gonorrhoea. The objective of the study is to identify the phytochemical responsible to cure the disease. *Filipendula ulmaria* contains"2-hydroxycalcone, 4-hydroxycalcone, L-ascorbic acid, vaniline, avicularin, salicin, rutin, spiraeoside, etc. "etc. These phytochemicals mightact against Covid-19. However, there is no such study available. This objective of the study is to identify the phytochemical of *filipendula ulmaria* capable of curing Gonorrhea.

MATERIALS AND METHODS

"Discovery studio module of Biovia software (Dassault Systemes of France)" was used for molecular docking. Published works showed that *filipendula ulmaria* contains"2-hydroxycalcone, 4-hydroxycalcone, L-ascorbic acid, vaniline, avicularin, salicin, rutin, spiraeoside,"etc.It was described in ancient medicinal systemscapable of controlling Corona disease.

Corona disease is caused by *SARS CoV-2*. It has been found from "Brenda enzyme database" that 6W4B is important tin microbial life cycle. Molecular docking was performed using the method described by Das et al. [4].High positive values of "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" presented a good interaction between the ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

RESULTS AND DISCUSSION

"CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm. It is a grid-based molecular docking method and optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods" [4]. Table 1 shows 6W4B-L-4-hydroxycalcone interaction was found to have the highest interaction.

CONCLUSIONS

Traditional medicines suggested that *filipendula ulmaria* plant has medicinal action against COVID-19 caused by SARS CoV-2. Using "Discovery studio module of Biovia software", molecular docking operation was performed. This study could explain that the presence of 4-hydroxycalcone is responsible for the action of *filipendula ulmaria* against 6W4B protein of corona virus.

REFERENCES

1. J Henrich, S Heine, A Norenzayan. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X
2. I. Hussain, R. Ullah, R. Ullah, M.Khurram, N. Ullah, A.Basee , F. Khan, M.Khattak, M. Zahoor, J. Khan, Dr. N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
3. P.Arulselvan, G.Karthivashan, S.Fakurazi,Journal of Chemical and Pharmaceutical Research 5 (7), 233-239, 2013
4. D. Das, S. Das, M. Pandey, D. Bhattacharyay. In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis, European Journal of Medicinal Plants, 2020.

Table 1. Results of C Docking

Sl No	Ligand	- C Docker Energy	- C Docker Interaction Energy	Difference Between - C Docker Interaction Energy and - C Docker Energy	Remarks
1	2-hydroxycalcone	-28.0804	0.92294	29.0033	
2	4-hydroxycalcone	9.2114	18.6557	9.4443	**Maximum inhibition of microbial enzyme**
3	L-ascorbic acid	3.98308	25.3160	21.3329	
4	Vaniline	17.8953	23.7539	5.8586	
5	Avicularin	FAILED	FAILED	FAILED	
6	Salicin	FAILED	FAILED	FAILED	
7	Rutin	FAILED	FAILED	FAILED	
8	Spiraeoside	FAILED	FAILED	FAILED	

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RESEARCH ARTICLE

In silico Analysis of Phytochemicals from *Mucuna pruriens* against COVID-19

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ABSTRACT

Phytochemicals from *Mucuna pruriens* plant extract can treat COVID-19. It is caused by *SARS CoV-2*. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDocker energy and -CDocker interaction energy"suggested that Dopamine can effectively deactivate the nucleocapsid protein N-terminal RNA binding domain (6M3M)enzyme thereby interrupting the life cycle of the organism.

Keywords: phytochemical, 6M3M, Discovery studio,*Mucuna pruriens*,*SARS CoV-2*

INTRODUCTION

Nature is a major source of medicines[1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action[2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Mucuna pruriens* belongs to family Fabaceae. Its extract is used to cure disease like COVID-19. The objective of the study is to identify the phytochemical responsible to cure the disease.*Mucuna pruriens* contains"dopamine, behenic acid, genistine and tannic "etc.These phytochemicals mightact againstCOVID-19. However, there is no such study available. This objective of the study is to identify the phytochemical of *Mucuna pruriens* capable of curing Corona disease.

MATERIALS AND METHODS

"Discovery studio module of Biovia software (Dassault Systemes of France)" was used for molecular docking. Published works showed that *Mucuna pruriens* contains"dopamine, behenic acid, genistine and tannic etc"etc.It was described in ancient medicinal systemscapable of controlling COVID-19. COVID-19is caused by SARS CoV-2. It has been found from "Brenda enzyme database" that nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme is important in viral life cycle.

Molecular docking was performed using the method described by Das et al. [4].High positive values of "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" presented a good interaction between the ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

RESULTS AND DISCUSSION

"CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm. It is a grid-based molecular docking method and optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods" [4]. Table 1 shows that 6M3M–Dpamine interaction was found to have the highest interaction.

CONCLUSIONS

Traditional medicines suggested that *M. pruriens* plant has medicinal action against COVID-19 caused by *SARS CoV-2.* Using "Discovery studio module of Biovia software", molecular docking operation was performed. This study could explain that the presence of Dopamine responsible for the action of *M. pruriens* against COVID-19 caused by SARS CoV-2.

REFERENCES

1. J Henrich, S Heine, A Norenzayan. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X
2. I. Hussain, R. Ullah, R. Ullah, M.Khurram, N. Ullah, A.Basee , F. Khan, M.Khattak, M. Zahoor, J. Khan, Dr. N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
3. P.Arulselvan, G.Karthivashan, S.Fakurazi,Journal of Chemical and Pharmaceutical Research 5 (7), 233-239, 2013
4. D. Das, S. Das, M. Pandey, D. Bhattacharyay. In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis, European Journal of Medicinal Plants, 2020.

Table 1. Results of C Docking

Sl No	Ligand	- C Docker Energy	- C Docker Interaction Energy	Difference Between - C Docker Interaction Energy And - C Docker Energy	Remarks
1	Dopamine	17.1475	16.5162	0.6313	Maximum inhibition of microbial enzyme
3	Behenic acid	failed	failed		
4	Genistine	-0.375823	35.0566	35.432423	
5	Tannic	failed	failed		

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RESEARCH ARTICLE

In silico Analysis of Phytochemicals from *Velvet bean* against Covid-19

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ABSTRACT

Phytochemicals from velvet bean plant extract can treat COVID-19.This disease mainly transmitted through or caused by a pathogenic virus known as SARS CoV-2. Molecular docking method applied using "Biovia Discovery Studio". "High positive values of -CDocker energy and -CDocker interaction energy"suggested that dopamine can effectively deactivate the protease 6Y2E enzyme thereby interrupting the life cycle of the organism.

Keywords: phytochemical, COVID-19, Discovery studio, Velvet bean,6Y2E

INTRODUCTION

Nature is a major source of medicines[1]. The medicinal value of the plants is due to the phytochemicals present in it. Phytochemicals can be derived from different parts of plants.Different medicinal plants and their phytoextracts have shown anti-microbial action[2]. These medicinal plants play a key role in human health care. Many people rely on the use of traditional medicine [3]. *Velvet bean* belongs to family Fabaceae. Velvet bean extract is used to cure disease like Gonorrhoea. The objective of the study is to identify the phytochemical responsible to cure the disease. *Velvet bean* contains "Dopamine and behenic acid"etc. These phytochemicals might act against COVID-19. However, there is no such study available. This objective of the study is to identify the phytochemical of Velvet bean capable of curing Corona disease.

MATERIALS AND METHODS

"Discovery studio module of Biovia software (Dassault Systemes of France)" was used for molecular docking.
Published works showed that Velvet bean contains"Dopamine and Behenic acid"etc.It was described in ancient medicinal systemscapable of controlling COVID-19. COVID-19 disease is caused by apathogen called as SARSCoV-2.. It has been found from "Brenda enzyme database" that main protease 6Y2E is important in viral life cycle.
Molecular docking was performed using the method described by Das et al. [4].High positive values of "-CDOCKER_ENERGY" and "-CDOCKER_INTERACTION_ENERGY" presented a good interaction between the

ligand and the receptor. Thus, the interactions with high values might indicate the major phytochemical responsible for curing the disease.

RESULTS AND DISCUSSION

"CDOCK is a molecular dynamics (MD) simulated-annealing-based algorithm. It is a grid-based molecular docking method and optimized for accuracy. The ligand conformations were obtained by Molecular Dynamic methods" [4]. Table 1 shows Protease CY2E enzyme--Dopamine interaction was found to have the highest interaction.

CONCLUSIONS

Traditional medicines suggested that **Velvet bean** plant has medicinal action against COVID-19 caused by SARSCoV-2.. Using "Discovery studio module of Biovia software", molecular docking operation was performed. This study could explain that the presence of dopamine is responsible for the action of **Velvet bean** against protease (6Y2E) of COVID-19 caused by SARSCoV-2.

REFERENCES

1. J Henrich, S Heine, A Norenzayan. The weirdest people in the world? Behavioral and Brain Sciences. 2010;33(2-3):61-83. DOI:10.1017/S0140525X0999152X
2. I. Hussain, R. Ullah, R. Ullah, M.Khurram, N. Ullah, A.Basee , F. Khan, M.Khattak, M. Zahoor, J. Khan, Dr. N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. 2011;10: 7487-7492.
3. P.Arulselvan, G.Karthivashan, S.Fakurazi,Journal of Chemical and Pharmaceutical Research 5 (7), 233-239, 2013
4. D. Das, S. Das, M. Pandey, D. Bhattacharyay. In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis, European Journal of Medicinal Plants, 2020.

Table 1. Results of C Docking

Sl No	Ligand	- C Docker Energy	- C Docker Interaction Energy	Difference Between - C Docker Interaction Energy and - C Docker Energy	Remarks
1	Dopamine	10.8994	13.9172	3.0178	Maximum inhibition of microbial enzyme
2	behenic acid	Failed	Failed	-	

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RESEARCH ARTICLE

Use of *Azolla pinnata* in the Diet of Laying Hen

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ABSTRACT

Nutrient content of fresh and dry *Azolla* was evaluated using different methods. Seventy Isa-brown pullets were distributed into diets; D_1 (control), D_2 (4% *Azolla*) and D_3 (8% *Azolla*), and reared in individual cages with standard management up to 44 weeks of age to investigate egg production. A total of 144 experimental (E), 32 (E and commercial farming -D_4), and 8 (E and D_4) eggs were tested to evaluate egg quality, DM, and yolk cholesterol, respectively. Fresh *Azolla* contained 3.64% DM and 96.36% moisture. Dry *Azolla* contained 23.44% crude protein, 2391.56 kcal/kg, 1.16% Ca, 1.29% P, 24.49% crude fiber and 32.70% ash. Diet D_2 and D_3 performed better than D_1 in terms of increased egg production, egg weight, yolk color, and Haugh unit. Diet D_3 showed the darkest yellow yolk color ($p<0.001$), followed by D_2 and D_1, respectively. Egg mass, FCR, and other egg quality traits were almost similar among the diets ($p>0.05$).Net-profit was tended to be higher with D_3, followed by D_2 and D_1, respectively. Body weight, feed intake, egg and egg mass production, and net-profit were increased with the increased age ($p<0.001$). The highest amount of DM was measured in D_2, followed by D_3, D_1, and D_4, respectively. The lowest amount of cholesterol ($p<0.001$) was determined in D_3, followed by D_2, D_1, and D_4, respectively. Hence commercial farming eggs (D_4) showed the lowest in quality in terms of DM and yolk cholesterol content. Therefore,8% of *Azolla* improved egg quality, yolk color, net-profit, and reduced yolk cholesterol.

Keywords: *Azolla*, cholesterol, dry matter, egg production, egg quality, hen.

INTRODUCTION

The poultry industry demands quality chicks, and good quality feed to support maximum production with a minimum production cost to get the maximum profit. Farmers are randomly using unexpected growth promoters, antibiotics, hormones, enzymes, and heavy metals to get rapid growth as well as more profits, which have a seriously harmful effect on poultry as well as on human health. Considering these facts, poultry scientists are trying to introduce alternatives in the diet of poultry to produce safe and profitable poultry products (1). A study (2) suggested using 15.7%, and 11% velvet bean replacing soybean meal in broiler starter, and finisher diet, respectively. *Azolla* reduced mortality, production cost, blood cholesterol, and increased profitability of broiler chicken (3).

Azolla (*Azolla pinnata*) is a small aquatic fern that floats on the surface of the water and forms a symbiotic relationship with the blue-green algae *Anabaena Azollae* located in the cavity of *Azolla* leaf. It can assimilate and fix atmospheric nitrogen, and convert to plant nitrogen. That is why *Azolla* is rich in protein, essential amino acids (lysine, leucine, arginine, and valine), vitamins (vita A, vita B_{12} and Beta carotene), chlorophylls and minerals like Ca, P, K, Fe, Mg, Mn, Cu, Zinc, Na, etc. *Azolla* is easy to cultivate or available in pond, roadside ditches, fallow land, lake, and paddy field. After harvesting, it is dried in the sun to grind and use in poultry diet as the cheap and abundant unconventional plant protein feed ingredient. *Azolla* improved feed conversion efficiency, energy efficiency, and economic performance without any deleterious effects on chickens as well as in the human body (4, 5,6). Several investigators showed increased egg production, feed conversion efficiency, profitability, and no mortality of laying hen fed diet with 5% *Azolla* (7, 8,9, 10). *Azolla* can increase body weight, and reduced cholesterol in the blood of broiler chicken (11, 12). A study (13) reported increased body weight and immunities of broiler chickens with 7.5% *Azolla* in the feed. A feeding trial to replace 20% commercial feed of chickens by fresh *Azolla* (14). In addition, *Azolla* is important to serve as a source of pigment for egg yolk and broiler skin (15). The deep yellow egg yolk color is appeared due to the presence of carotenoids (yellow: lutein and zeaxanthin) deposited in *Azolla* leaf meal which safely interacts with free radical as an antioxidant, and terminate the chain reaction before vital molecules are damaged, ultimately prevent cancer, and improve the immune function of the body. Yolk coloration is also responsible to produce Omega-3 fatty acid-enriched eggs, which reduce triglyceride as well as reduce the risk of heart disease. Carotenoid eggs, even sell at a higher price. A recent study in Beijing reported that for every unit increase in YolkFan™, the price was increased by 0.18 RMB (US$ 0.025) per egg. Similarly, in India or other countries, the yolk is displayed on the external surface of the package of the egg (16). Besides all of those, *Azolla* plays a vital role to reduce the cholesterol of egg yolk.

A few scattered works have been done using *Azolla* in the diet of laying hen for assessing egg production, and egg quality. But no literature of particular concern was found, assessing the effect of *Azolla* on dry matter, yolk color and cholesterol content of eggs. Therefore, the present study was planned for assessing the nutrient content of *Azolla*, and the effect of *Azolla* on egg production, profitability, egg quality, egg yolk color, and cholesterol content of egg for producing quality, safe and profitable chicken eggs.

MATERIALS AND METHODS

Approaches

Fresh and sun-dried *Azolla* were used to assess nutrient content. The field and Lab experiments were carried out with control (no *Azolla*), 4%, and 8% *Azolla* in the diet of laying hen at Bangabandhu Sheikh Mujibur Rahman Agricultural University (BSMRAU), Bangladesh to produce quality, safe and profitable eggs.

Collection and preparation of *Azolla* meal

Azolla pinnata was cultivated in fresh water ponds of BSMRAU, Gazipur, Bangladesh and then collected in every week, and dried in the sun to grind using a grinder machine. In addition, fresh *Azolla* was also collected from the paddy field, lake, roadside ditches, and fallow land, and then processed accordingly (Figure 1).

Nutrient analysis of *Azolla*

Nutritional composition of fresh and sun-dried *Azolla* was determined at the Lab of the Department of Dairy and Poultry Science (DM and moisture %), Department of Soil Science (CP, Ca, P, Mn, Mg), Department of Agro-processing (Energy), BSMRAU and the Department of Livestock Services (CF and total ash), Dhaka, Bangladesh. Thereafter, sun-dried *Azolla* was used in the diet of laying hens.

Feeding trial

A total of 70 ISA- brown ready to pullet was distributed into 3 dietary groups; D_1 (control-no *Azolla*), D_2 (diet with 4% *Azolla*), and D_3 (diet with 8% *Azolla*). The pullets were reared in an individual cage management system to measure laying performance, egg quality, egg dry matter, egg yolk color, and cholesterol content. The iso-nitrogenous and iso- caloric layer diet containing 17% CP and 2750 kcalME/kg were provided to the birds as per standard is given by the breeder (Table 1), and clean and fresh water *ad libitum*. The birds were exposed for 17 hrs lighting regime during the laying period. Body weight and feed intake were recorded fortnightly. The number of eggs was recorded daily. Egg quality traits; egg weight, albumen weight, width and height, yolk weight, width and height, eggshell weight, eggshell with membrane thickness, and yolk color were measured at 24, 28, 36 and 44 weeks of age of the bird. Dry matter of experimental, and commercial farming eggs was measured at 36 and 42 weeks of age of laying hen. Egg yolk cholesterol of experimental, and commercial farming eggs was measured at 36 weeks of age of the bird. The Roche yolk color fan was used to measure egg yolk color (Figure 1). Egg mass (g/bird), FCR (Feed/dozen or kg eggs), Haugh unit, yolk index and a specific gravity of egg were calculated. Production cost (Tk/dozen eggs) was calculated considering bird, feed, mortality and labor cost. Profitability (Tk/dozen eggs) was calculated from the sale and production cost of a dozen eggs.

Statistical analysis

The collected data were analyzed using the statistix10 computer package program. Cholesterol content of egg yolk was analyzed using a t-test.

Statistical model: The following statistical model was used for data analysis.

$Y_{ijk} = \mu + D_i + A_j + (D \times A)_{ij} + e_{ijk}$

Where,

Y_{ijk} is the observation of the kth number of individual birds in the ith dietary and jth age group.

μ is the overall mean

D_i is the fixed effect of the ith dietary group (i = 1……4)

A_j is the effect of the jth age group (j=1, 2 ……7)

e_{ijk} is the random error

RESULTS

Nutrient content of *Azolla* (*Azolla pinnata*)

Nutrient content of fresh and sun-dried *Azolla* (*Azolla pinnata*) is shown in Table 2. Fresh *Azolla* contained 3.64% dry matter and 96.36% moisture. Sun-dried *Azolla* contained 23.44% CP, 2391.56 KcalME/kg, 1.02% Ca, 0.40% P, 0.76% Mn, 2.05% Mg, 24.47% CF and 32.70% total ash.

Effect of *Azolla* on egg production performance, and net-profit of laying hen

Feed intake ($p<0.001$), egg production ($p<0.05$), egg weight ($p<0.001$) significantly differed among the dietary groups, but there was no significant difference among the diets considering body weight, egg mass, FCR, production cost and net profit ($p>0.05$). Age influenced body weight, feed intake, egg production, egg weight, egg mass and net profit ($p<0.001$) but didn't affect FCR and production cost ($p>0.05$). Diet and age interacted for feed intake ($p<0.001$), egg mass ($p<0.05$), FCR ($p<0.05$) and production cost ($p<0.01$), and not interacted for body weight, egg production, egg weight, and net profit ($p>0.05$) (Table 3).

An increasing trend of body weight was observed in diet D_3, followed by D_2 and D_1, respectively. The significantly increased body weight was found at 162 days compared to the 12 days of laying period but did not exceed the standard (ISA-brown) given by the breeder. The lowest feed intake was observed in diet D_3 with the highest egg weight and egg mass at 182 days of laying period, followed by D_1 and D_2, respectively. Feed intake was increased with the advancement of the laying period. Dietary groups showed the highest egg weight at 162 days of the laying period. The highest number of egg production was found in diet D_2 (153.36 eggs) at 182 days followed by D_3 (152.02 eggs) and D_1 (151.07 eggs), respectively. Evidently but not significantly, the highest egg mass production and the lowest FCR was observed in D_3 at 182 days, followed by D_2 and D_1, respectively. No mortality was found among the dietary groups during the experimental period. Cumulative egg mass production was increased with the increased age of birds. The production cost was tended to be decreased with the increased number of egg production, but the more decreasing tendency was observed at 162 and 182 days compared to 12 and 71 days of the production period. Evidently but not significantly, the lowest amount of production cost and the highest amount of net-profit was observed in the D_3 at 182 days followed by D_2 and D_1, respectively. The significant interaction of diet and age was found for egg production cost (Tk/dozen eggs). Therefore, D_3 performed the best in terms of body weight, feed intake, egg production, egg weight, egg mass, FCR, and net-profit.

Effect of *Azolla* on egg quality traits of laying hen

Egg quality traits are shown in Table 4. Albumen height, yolk color (pigmentation) and Haugh unit significantly differed among dietary groups ($p<0.001$). The other egg quality traits were almost similar between the dietary groups ($p>0.05$). There was no age effect on yolk height, yolk/albumen ratio, eggshell weight, yolk index and specific gravity ($p>0.05$), but age affected egg weight, albumen weight, albumen width ($p<0.001$), albumen height ($p<0.05$), yolk weight ($p<0.001$), yolk width ($p<0.01$), eggshell with membrane thickness, yolk color ($p<0.001$), and Haugh unit ($p<0.05$). The egg quality traits were increased or tended to be increased with the increased age of the bird, except the traits; eggshell with membrane thickness, yolk index, and specific gravity. Those had a tendency to decrease with the increasing age of birds. The diet and age interacted for albumen width ($p<0.05$), eggshell with membrane thickness ($p<0.01$), and yolk color ($p<0.001$), but not interacted for other egg quality traits ($p>0.05$). The highest albumen height and Haugh unit were observed in D_2, followed by D_3 and D_1, respectively. The other egg quality traits tended to be higher in D_2 followed by D_3 and D_1, respectively. However, the deepest yellow yolk color was measured in D_3 followed by D_2 and D_1, respectively. Therefore, *Azolla* significantly enhanced egg yolk color compared to the control diet (D_1). of the two diets, 8% *Azolla* was much better than 4% in terms of increasing egg yolk color. Evidently but not significantly, the lowest yolk/albumen ratio was observed in D_3, followed by D_2 and D_1, respectively.

Dry matter content of egg of laying hen fed diets with 4% or 8%*Azolla*, and commercial farming eggs

The significant difference was observed among dietary groups for the traits of egg weight ($p<0.05$), DM and moisture content of egg ($p>0.05$) (Table 5). The highest egg weight and DM%, and the lowest moisture% were determined in D_3, followed by D_1, D_2, and D_4 (Commercial farming eggs), respectively. No effect of age and interaction of diet and age on egg weight, DM and moisture content of the egg was observed ($p>0.05$). However, age group A_1 (36 weeks of age of the bird) was tended to be better than A_2 (42 weeks of age of the bird) in terms of DM and moisture content of the egg.

Cholesterol content of egg yolk of laying hen fed diets with 4% or 8% *Azolla*, and commercial farming eggs

The highly significant difference was found among the diets for the cholesterol content of egg yolk ($p<0.001$). The lowest amount of cholesterol was measured in D_3, followed by D_2, D_1, and D_4, respectively. Therefore, *Azolla* reduced cholesterol in egg yolk, and the reduction trend was more in D_3 compared to D_2. Commercial farming eggs showed the highest amount of cholesterol (263.98 mg) among the dietary groups (Table 6).

DISCUSSION

Nutrient content of *Azolla* (*Azolla pinnata*)

The estimated DM (3.64%) of fresh *Azolla* in the present study was lower than 4.70% reported by Anitha et al. (17). The values of CP% (23.44%) and energy (2391.56 kcal/kg) in sun-dried *Azolla* measured in the study were higher than the values reported by several investigators (7,17,18) but corroborated the values reported by Cherry et al. (19). They found 23.49% CP and 24.26% total ash, and Khatun et al. (7) found 21.9% CP and 1812.83 KcalME/kg in *Azolla*. The estimated values of CF (24.49%) and total ash (32.70%) in the present study were higher than the values reported by several investigators (19,17). Anitha et al. (17) reported 14.70% CF and 17.34% ash in *Azolla*. The evaluated calcium (1.02%) and phosphorus (0.402%) in the study were consistent with the findings of Sujatha et al. (6), and partially supported Alalade and Lyayi (9). They reported 1.16% Ca and 1.29% P in *Azolla* of which P% was higher than the present study. A study showed (17) the 2.03% Ca and 0.59% P in *Azolla* which were higher than the present study. The values of Mn (0.76%) and Mg (2.05%) in the present study were higher than the findings reported by several investigators (17,6). Therefore, *Azolla* (*Azolla pinnata*) as an unconventional natural protein source feed item may include in the diet of poultry.

Effect of *Azolla* on egg production performance, and net profit of laying hen

Body weight was similar among the diets within the age group but was increased at 162 days compared to the 12th day of the laying period. However, body weight did not exceed the standard given by the breeder. The lowest feed intake was observed in D_3 followed by D_1 and D_2, respectively. Birds in test diets (D_2 or D_3) laid the higher number of eggs at 182 days compared to the control diet (D_1). The number of egg production was statistically similar between the test diets. Egg weight and egg mass production were increased with the increase of bird age. Moreover, the highest egg weight was observed in D_3 followed by D_2 and D_1, respectively. The feed conversion ratio (FCR) on dozen of eggs or on egg mass production at 182 days of laying period was tended to lower in diet D_3 followed by D_1 and D_2, respectively. The above findings were supported by Alalade et al. (10). There was a tendency to decrease in production cost, and increase in net profit in test diets at 182 days of the production period compared to control diet because of increased egg and egg mass production which was consistent with the findings reported by Nagashi et al. (20). Of the test diets, D_3 performed better than D_2 in terms of production cost and net profit supported Khatun et al. (7).

Body weight, feed intake, egg production, egg weight, egg mass production, and net profit were influenced by age of the bird. There was a tendency to decrease in FCR, and production cost with the increased age of birds because of increased egg and egg mass production. This is why net profit was increased with the increase of bird age. Interaction between diet and age was observed for feed intake, egg weight, egg mass, FCR, and production cost.

Effect of *Azolla* on egg quality traits of laying hen

Egg quality traits were statistically similar among dietary groups except for albumen height, yolk color, and Haugh unit. However, albumen weight, yolk weight, and height, eggshell with membrane weight and thickness, yolk index, and specific gravity were tended to be increased in D_2 and D_3 at 44 weeks of bird age compared to D_1. of the test diets, D_2 performed better than D_3 for these traits. There was a tendency to decrease in albumen width, and yolk/albumen ratio with D_3 followed by D_2 and D_1, respectively. Albumen width is related to the freshness of an egg, and the lower albumen width indicates the higher albumen firmness as well as the freshness of the egg. Accordingly,

albumen and yolk height indicate the freshness of eggs as well as the quality of the egg. Albumen width and height also indicate the quantity of protein in the egg. Lower yolk/albumen ratio indicates the smaller yolk, and larger albumen size that implies the increasing quantity of egg protein, and reduce the fat as well as cholesterol content of egg yolk. Considering these facts, the best quality egg was found in D_2 in terms of higher height, and lower width of albumen and yolk, followed by D_3 and D_1, respectively. However, D_3 performed the best; for increasing yolk color, followed by D_2 and D_1, respectively. *Azolla* was responsible for the increasing yolk color. The deepest yellow yolk color was appeared on adding higher-level *Azolla* with laying hen diet. *Azolla* leaf contained Vit-A and Beta carotene-rich in lutein and Zeaxanthin which was responsible for yolk coloration, corroborated the findings of Khatun et al. (7). These carotenoids (yellow) act as antioxidants that can prevent cancer, heart disease, and improve the immune function of the body. The highest amount of albumen, and eggshell with membrane thickness was observed at 28 weeks of age compared to the other age groups which imply; the suitable age group for producing quality eggs. The other egg quality traits were increased or tended to be increased with increasing bird age. The highest level of yolk color was observed at 44 weeks of bird age. The interaction between diet and age was found in albumen width, eggshell with a membrane thickness, and yolk color.

Dry matter content of egg of laying hen fed diets with 4% or 8% *Azolla*, and commercial farming eggs

Literature related to the effect of *Azolla* on the dry matter content of a chicken egg is still not available. The highest DM% and the lowest moisture% were determined in eggs of D_2 (4% *Azolla*) or D_3 (8% *Azolla*) among the dietary groups. Diet D_2 and D_3 were almost similar for containing DM and moisture in the egg. Commercial farming eggs (D_4) showed the lowest DM% and the highest moisture%. Although the control diet (D_1) was poorer than D_2 or D_3, but better than D_4 in terms of DM and moisture content of the egg. Hence, commercial farming eggs were the lowest in quality in terms of DM content. Therefore, *Azolla* increased DM of the egg.

Cholesterol content of egg yolk of laying hen fed diets with 4% or 8% *Azolla*, and commercial farming eggs

In the present study, commercial farming eggs (D_4) showed the highest cholesterol level (263 mg/egg), followed by 237 mg, 210 mg, and 201.93 mg cholesterol in D_1 (control), D_2 (4% *Azolla*), and D_3 (8% *Azolla*), respectively. Estimated cholesterol levels in commercial farming eggs and egg of control diet exceeded the level of cholesterol reported by Spence et al. (21). They reported 215 - 213 mg cholesterol in a standard size egg (56-58g/egg). Estimated egg yolk cholesterol level was found to be lower in the diet with 4% or 8% *Azolla* than the reference level, supported by Balaji et al. (12). However, the egg of D_3 contained much lower level cholesterol than D_2 (4% *Azolla*). Therefore, D_3 was the best performer dietary group in terms of cholesterol reduction in egg yolk. No previous work to estimate the effect of *Azolla* on the cholesterol content of egg of laying hen was found. The diet D_2 also performed better than D_1 or D_4 (Commercial farming eggs) in terms of the cholesterol content of the yolk. *Azolla* reduced blood cholesterol of broiler chicken reported by several investigators (11,3) which also supported the present findings. Therefore, *Azolla* reduced egg yolk or blood cholesterol. It may be a novel and beneficial feed item in the diet of poultry.

CONCLUSION

The present study reveals that *Azolla* is rich in protein, energy, vitamins, and minerals. Either 4% **(D_2)** or 8% *Azolla* **(D_3)** may be used in the diet of laying hen because of increased egg production, survivability, egg quality, net profit, and significant reduction of cholesterol in egg yolk. Both the percentage of *Azolla* (D_2 and D_3) incredibly performed better than D_1 in terms of yolk coloration. Diets containing *Azolla* were superior to control or D_4 (commercial farming eggs) because of contained an increased amount of DM, and reduced cholesterol levels in egg yolk. However, the diet containing 8% *Azolla* was better than 4% *Azolla* in terms of increased egg, and egg mass production, net profit, yolk/albumen ratio, yolk color, and reduced yolk cholesterol. The other egg quality traits were statistically similar between D_2 and D_3. The 8% *Azolla* may be the most beneficial to include in the diet of laying hen for producing quality, safe and profitable eggs. Therefore, *Azolla* may be a novel feed item in the diet of poultry.

However, more studies are needed to confirm these findings as well as to measure the digestibility of *Azolla*, and the effect of *Azolla* on the hematological condition, lipid profiles, and immunity of birds.

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ETHICAL STATEMENTS

This study was approved by the Institutional Committee on Animal Care and Use in Research (ICACUR), BSMRAU, and carried out following the Guidelines for Experimental Animals (Livestock and Poultry) of the Ministry of Livestock and Fisheries (Dhaka, Bangladesh).

REFERENCES

1. Almeida AM de, Zuber U. The effect of Naked Neck genotype (Nana), feeding and outdoor rearing on growth and carcass characteristics of free range broilers in a hot climate. Tropical Animal Health and Production. 2010; 42: 99-107.
2. Vadivel V, Pugalenthi M. Studies on the incorporation of velvet bean (*Mucuna pruriens* var. *utilis*) as an alternative protein source in poultry feed and its effect on growth performance of broiler chickens. Tropical Animal Health and Production. 2010; 42: 1367- 1376.
3. Islam MA, Nishibori M. Use of multivitamin, acidifier and *Azolla* in the diet of broiler chickens. Asian-Australasian Journal of Animal Sciences. 2017;30: 683-689.
4. Lejeunea A, Cagauana A, Vanhove C.*Azolla* research and development of recent trends and properties. Symbiosis. 1999;27: 333-351.
5. Namra MMM, Hataba NA, Wahed M. The productive performance of growing chicks fed restricted diets supplemented with free *Azolla*. Egyptian Poultry Science. 2010; 30: 747-762.
6. Sujatha T, Udhayakumar D, Kundu A, Jeyakumar S, Jai Sundar, Kundu MS.Utilization of raw *Azolla* as a natural feed additive for sustainable production in Nicobari fowl. Animal Science Reporter. 2013;7: 146-152.
7. Khatun A, Ali MA, Dingle JG. Comparison of the nutritive value for laying hens of diets containing *Azolla* (*Azolla pinnata*) based on formulation using digestible protein and digestible amino acid versus total protein and total amino acid. Animal Feed Science and Technology. 1999; 81: 43-46.
8. Basak B, Pramanik MAH, Rahman MS, Tarafdar SU, Roy BC.*Azolla* (*Azolla pinnata*) is a feed ingredient in broiler ration. International Journal of Poultry Science. 2002;1(1)**:** 29-34.
9. Alalade OA, Lyayi EA**.** Chemical composition and the feeding value of *Azolla* (*Azolla pinnata*) meal for egg type chickens. International Journal of Poultry Science.2006;5(2): 137-141.
10. Alalade OA, Iyayi EA, Alalade TO. The nutritive value of *Azolla* (*Azolla pinnata*) meal in diets for growing pullets and subsequent effect on laying performance. Journal of Poultry Science.2007; 44: 273-277.
11. Balaji K, Jalaludeen A, Richard C R, Peethambaran PA, Senthilkumar S.Effect of dietary inclusion of *Azolla* (*Azolla pinnata*) on production performance of broiler chicken. Indian Journal of Poultry Science. 2009; 44(2): 195-198.
12. Balaji K, Jalaludeen A, Kannan A. Effect of dietary *Azolla* on cholesterol content in broiler chicken. Indian Veterinary Journal. 2010;87 (5): 478-480.
13. Prabina BJ, Kumar K. Dried *Azolla* as a nutritionally rich cost effective and immune modulatory feed supplement for broilers. The Asian Journal of Animal Science. 2010; 5: 20-22.

14. Subudhi BPR, Singh PK. Nutritive value of the water fern *Azolla pinnata* for chicks. Poultry Science.1978; 57**:** 378-380.
15. Maurice DV, Jones JE, Dillon CR, Weber JM. Chemical composition and nutritional value of Brazilian Elodea (*Egeriadensa*) for the chick. Poultry Science. 1984;63: 317-323.
16. DSM in Animal Nutrition and Health. Pigmenting egg and broiler chickens. 2016;http://www.dsm.com/markets/anh/en-US
17. Anitha KC, Rajeshwari YB, Prasanna SB, Shree Shilpa J.Nutritive evaluation of *Azolla* as Livestock. Journal of Experimental Biology and Agricultural Science. 2016; 4:Doi:http://dx.doi.org/10.18006/2016.4 (Issue6).670.674.
18. Boitai SS, Babu LK, Panda AK, Mohapatra L, Sahoo B. Effect of dietary incorporation of *Azolla* meal on production performance and quality of Vanarja laying hens. International Journal of Livestock Research. 2018; 8: 264-270.
19. Cherry DM, Prasad RMV, Jagadeeswararao S, Jayalaxmi P, Kumar D Srinivaas. A study on the nutritive value of *Azolla pinnata*. Livestock Research International. *2014;* 2: 13-15.
20. Nagashi H, Khojasteh S, Jafari M. Investigation of the effect of different levels of *Azolla* (*Azolla pinnata*) on performance, and carcass characteristics of Cobb broiler chicks. International Journal of Farming and Allied Science. 2014; 3**:** 45-49.
21. Spence JD, Jenkins DJA, Davignon V. Dietary cholesterol and egg yolk: Not for patients at risk of vascular disease. The Canadian Journal of Cardiology. 2010; 26: e-336-339.

Table 1.Composition of diets used in the experiment

Ingredients	**Amounts (kg)**		
	D_1	**D_2**	**D_3**
Maize	59.50	64.50	62.50
Soybean meal	22.00	20.50	18.50
Rice polish	7.00	-	-
Protein concentrate	3.00	3.00	3.00
Azolla	---	4.0	8.0
Limestone	8.00	7.50	7.50
Salt	0.50	0.50	0.50
Total	100.00	100.00	100.00
Calculated composition:			
Crude protein (CP)%	17.32	17.21	17.03
ME Kcal/kg	2770.08	2766.69	2737.26
Ca%	3.32	3.08	3.12
Av. P%	1.09	0.43	0.46
Lysine%	0.95	1.04	0.99
Methionine%	0.49	0.49	0.41

•D_1 = Control diet (No *Azolla*); D_2= Diet with 4% *Azolla*; D_3 = Diet with 8% *Azolla*

Table 2.Nutrient content of *Azolla* (*Azolla pinnata*)

Nutrient	Amount
Dry matter (DM) (%) (Fresh basis)	3.64
Moisture (%) (Fresh basis)	96.36
Crude protein (CP) (%)	23.44
Energy (ME Kcal/kg)	2391.56
Ca (%)	1.02
Av. P (%)	0.40
Mn (%)	0.76
Mg (%)	2.05
Crude fibre (CF) (%)	24.47
Total ash (%)	32.70

•Crude protein, Energy, Ca, Mg, P and Mn were estimated following micro-Kjeldhal method, Oxygen bomb calorimetric method, NH4OAC extraction method, Bray and Kurtz method and DTPA extraction method, respectively.

Table 3.Egg production performances of laying hen fed diets with 4% or 8% *Azolla* up to 182 days of the laying period

Traits	Diet (D)	Age (A)								LSD value and level of significance+		
		12d	43d	71d	101d	132d	162d	182d	Mean	D	A	D x A
Body weight (g/bird)	D_1	1598.50					1703.50		1651.00	109.170^{NS}	77.378^{***}	154.380^{NS}
	D_2	1621.90					1754.60		1688.30			
	D_3	1641.60					1831.20		1736.40			
	Mean	1620.70					1763.10		1691.90			
Feed intake (g/bird)	D_1	880.00	3406.00	7119.00	10599.00	13730.00	16954.00	19494.00	10312.00	117.32^{***}	155.57^{***}	158.58^{***}
	D_2	686.00	3591.00	7170.00	10392.00	13725.00	17289.00	20609.00	10495.00			
	D_3	664.00	3610.00	7239.00	10381.00	13637.00	17051.00	18973.00	10222.00			
	Mean	743.00	3536.00	7176.00	10457.00	13697.00	17097.00	19692.00	10343.00			
Egg production (No./bird)	D_1	5.17	31.72	57.30	84.09	108.30	134.52	151.07	81.739	2.714^{*}	3.599^{***}	3.667^{NS}
	D_2	6.77	32.19	55.52	81.19	106.02	134.36	153.36	81.346			
	D_3	4.02	26.86	51.19	78.02	104.36	133.02	152.02	78.501			
	Mean	5.32	30.26	54.67	81.10	106.23	133.97	152.15	80.53			
Egg weight (g/egg)	D_1	50.44	50.69	51.99	52.06	51.40	55.03	54.72	52.33	1.109^{***}	1.471^{***}	1.499^{NS}
	D_2	53.27	52.68	52.56	54.01	55.02	58.24	54.04	54.26			
	D_3	52.87	52.59	52.84	52.09	55.83	58.97	57.50	54.67			
	Mean	52.20	51.98	52.47	52.72	54.08	57.42	55.42	53.76			
Egg mass (g/bird)	D_1	259.70	1604.60	2985.00	4379.70	5552.30	7398.70	8265.20	4349.30	173.02^{NS}	229.43^{***}	233.80^{*}
	D_2	329.60	1664.60	2903.00	4379.70	5552.30	7398.70	8265.20	4454.40			
	D_3	181.70	1383.1	2674.50	4040.00	5798.70	7809.30	8699.00	4369.50			
	Mean	257.00	1550.80	2854.10	4263.00	5715.50	7673.80	8423.20	4391.10			
FCR /dozen eggs	D_1	2797.00	1392.00	1518.80	1531.90	1543.50	1533.10	1568.90	1697.90	318.21^{NS}	421.97^{NS}	430.010^{*}
	D_2	1607.00	1514.40	1686.30	1618.00	1606.80	1585.20	1647.00	1609.2			
	D_3	1568.20	1834.40	1806.80	1661.20	1614.40	1568.00	1520.50	1653.40			
	Mean	1990.70	1580.30	1670.60	1603.70	1588.20	1562.10	1578.80	1653.50			
FCR /kg egg	D_1	4.67	2.32	2.45	2.46	2.52	2.33	2.40	2.74	0.546^{NS}	0.724^{NS}	0.738^{*}
	D_2	2.55	2.38	2.67	2.48	2.42	2.25	2.53	2.46			
	D_3	3.27	2.52	2.65	2.53	2.44	2.26	2.37	2.58			
	Mean	3.27	2.53	2.65	2.53	2.44	2.26	2.37	2.58			
Production cost (Tk/dozen eggs)	D_1	90.12	54.83	58.16	58.50	58.81	58.53	59.47	62.63	8.550^{NS}	11.338^{NS}	11.554^{**}
	D_2	55.46	56.20	60.48	58.78	58.50	57.97	59.50	58.13			
	D_3	48.15	62.10	61.44	57.98	56.87	55.76	54.64	56.70			
	Mean	64.57	57.71	60.03	58.42	58.06	57.42	57.87	59.15			
Net-profit (Tk/dozen eggs)	D_1	-13.42	29.17	25.84	25.49	25.19	25.47	24.52	20.32	7.700^{NS}	10.211^{***}	10.405^{NS}
	D_2	15.49	28.75	24.47	26.17	26.45	26.99	25.45	24.83			
	D_3	1.80	22.85	23.51	26.97	28.08	29.19	30.32	23.25			
	Mean	1.29	26.92	24.61	26.21	26.57	27.21	26.76	22.80			

+NS, p>0.05; *, p<0.05; ***, p<0.001; d=days; D_1 = Control diet (No *Azolla*); D_2= Diet with 4% *Azolla*; D_3 = Diet with 8% *Azolla*

Table 4.Egg quality of laying hen fed diets with 4% or 8% *Azolla* at different ages of the bird

Traits	Diet (D)	Age (A) in week					LSD value and level of Significance+		
		24	28	36	44	Mean	D	A	D x A
Egg weight (g/egg)	D_1	50.88	54.29	55.26	57.02	54.366	1.829^{NS}	2.112^{***}	3.658^{NS}
	D_2	52.47	54.47	57.13	56.49	55.14			
	D_3	52.63	53.84	58.01	57.06	55.38			
	Mean	51.99	54.20	56.80	56.86	54.96			
Albumen weight (g/egg)	D_1	31.65	33.11	34.42	35.35	33.63	1.551^{NS}	1.791^{***}	3.102^{NS}
	D_2	32.83	33.62	35.22	37.01	34.67			
	D_3	33.16	33.18	36.09	35.21	34.41			
	Mean	32.55	33.31	35.24	35.86	34.24			
Albumen width (mm)	D_1	75.79	81.53	83.47	80.70	80.37	2.481^{NS}	2.865^{***}	4.963^{*}
	D_2	75.15	76.20	77.88	83.24	78.12			
	D_3	78.61	75.07	75.96	82.61	78.06			
	Mean	76.51	77.60	79.10	82.19	78.85			
Albumen height (mm)	D_1	9.50	9.56	9.75	9.87	9.67	0.563^{***}	0.650^{*}	1.126^{NS}
	D_2	10.95	11.57	11.36	10.41	11.08			
	D_3	10.07	11.57	11.27	10.08	10.75			
	Mean	10.17	10.90	10.79	10.12	10.50			
Yolk weight (g/egg)	D_1	12.30	13.76	14.26	14.35	13.67	0.946^{NS}	1.092^{***}	1.892^{NS}
	D_2	12.37	13.54	14.36	15.99	14.06			
	D_3	12.19	13.31	14.29	14.19	13.49			
	Mean	12.28	13.54	14.30	14.85	13.74			
Yolk width (mm)	D_1	37.48	38.48	39.64	39.39	38.75	1.195^{NS}	1.380^{**}	2.391^{NS}
	D_2	36.32	39.96	39.07	37.20	38.14			
	D_3	37.76	38.74	39.88	39.94	39.08			
	Mean	37.18	39.06	39.53	38.84	38.65			
Yolk height (mm)	D_1	14.72	14.23	14.69	14.83	14.62	0.325^{NS}	0.376^{NS}	0.651^{NS}
	D_2	14.88	15.16	15.22	14.59	14.97			
	D_3	14.97	15.11	14.98	14.24	14.83			
	Mean	14.86	14.83	14.97	14.55	14.80			
Yolk/Albumen ratio	D_1	0.393	0.425	0.422	0.411	0.413	0.026^{NS}	0.031^{NS}	0.053^{NS}
	D_2	0.380	0.403	0.408	0.433	0.406			
	D_3	0.369	0.402	0.401	0.408	0.395			
	Mean	0.381	0.401	0.411	0.417	0.404			
Egg shell with membrane weight (g/egg)	D_1	6.57	6.95	7.01	7.10	6.91	0.272^{NS}	0.314^{NS}	0.544^{NS}
	D_2	6.99	6.88	7.14	7.11	7.03			
	D_3	6.76	6.99	7.12	7.21	7.02			
	Mean	6.77	6.94	7.09	7.14	6.99			
Egg shell with membrane thickness (mm)	D_1	0.496	0.524	0.429	0.435	0.471	0.013^{NS}	0.015^{***}	0.026^{**}
	D_2	0.529	0.509	0.376	0.476	0.473			
	D_3	0.509	0.488	0.357	0.500	0.464			
	Mean	0.511	0.507	0.387	0.470	0.469			

Yolk color		**D_1**	**5.00**	**5.16**	**7.41**	**6.50**	**6.02**	0.480^{***}	0.554^{***}	0.960^{***}
		D_2	**10.58**	**12.08**	**10.67**	**12.08**	**11.35**			
		D_3	**13.33**	**14.25**	**12.92**	**14.00**	**13.63**			
		Mean	**9.64**	**10.50**	**10.33**	**10.86**	**10.33**			
Haugh unit		**D_1**	98.85	98.23	98.96	99.14	98.79	2.433^{***}	2.810^{*}	4.867^{NS}
		D_2	104.53	106.42	105.42	101.28	104.41			
		D_3	101.08	106.81	104.89	100.03	103.20			
		Mean	101.49	103.82	103.09	100.15	102.14			
Yolk Index		**D_1**	0.394	0.370	0.371	0.378	0.378	0.023^{NS}	0.027^{NS}	0.047^{NS}
		D_2	0.412	0.379	0.389	0.426	0.402			
		D_3	0.397	0.390	0.376	0.357	0.380			
		Mean	0.401	0.380	0.379	0.387	0.387			
Specific gravity		**D_1**	1.103	1.103	1.102	1.101	1.102	0.0028^{NS}	0.0033^{NS}	0.0057^{NS}
		D_2	1.106	1.102	1.101	1.101	1.103			
		D_3	1.103	1.104	1.099	1.101	1.102			
		Mean	1.104	1.103	1.101	1.101	1.102			

+NS, p>0.05; *, p<0.05; **, p<0.01; ***, p<0.01; D_1 = Control diet (No *Azolla*); D_2= Diet with 4% *Azolla*; D_3 = Diet with 8% *Azolla*

Table 5.Dry matter content of egg of laying hen fed diets with 4% or 8% *Azolla*, and commercial farming eggs at different ages

Traits	**Age (A)**	**Diet (D)**					**LSD value and level of significance+**		
		D_1	D_2	D_3	D_4	Mean	D	A	D x A
Egg weight (g/egg)	A_1	56.97	60.54	58.58	49.97	56.51	5.539^{*}	4.187^{NS}	7.253^{NS}
	A_2	56.35	59.20	58.06	53.15	56.68			
	Mean	56.66	59.87	58.32	51.56	56.60			
Egg dry matter (%)	A_1	30.87	34.27	33.17	28.84	31.78	1.757^{**}	1.328^{NS}	2.300^{NS}
	A_2	31.15	31.29	31.91	29.75	31.03			
	Mean	31.01	32.78	32.54	29.30	31.41			
Moisture content (%)	A_1	69.13	65.74	66.83	71.15	68.21	1.757^{**}	1.328^{NS}	2.300^{NS}
	A_2	68.85	68.71	68.09	70.24	68.97			
	Mean	68.99	67.22	67.46	70.70	68.59			

+NS, p>0.05; *, p<0.05; **, p<0.01; A_1 = 36 weeks of age of bird; A_2 = 42 weeks of age of bird, D_1 = Control diet (No *Azolla*); D_2= Diet with 4% *Azolla*; D_3 = Diet with 8% *Azolla*; D_4 =Commercial farming egg

Table 6.Cholesterol content of egg yolk of laying hen fed diets with 4% or 8% *Azolla*, and commercial farming eggs at 36 weeks of age of the bird

Diet (D)	Amount of egg yolk cholesterol (mg/100g)	t- value and level of significance+
D_1	237.18	t-14.149***
D_2	210.95	
D_3	201.93	
D_4 (Commercial farming egg)	263.98	

+ ***, p<0.001; Lab: Institute of Food Science and Technology, Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhanmondi, Dhaka-1205, Bangladesh; D_1 = Control diet (No *Azolla*); D_2= Diet with 4% *Azolla*; D_3 = Diet with 8% *Azolla*; D_4 =Commercial farming eggs

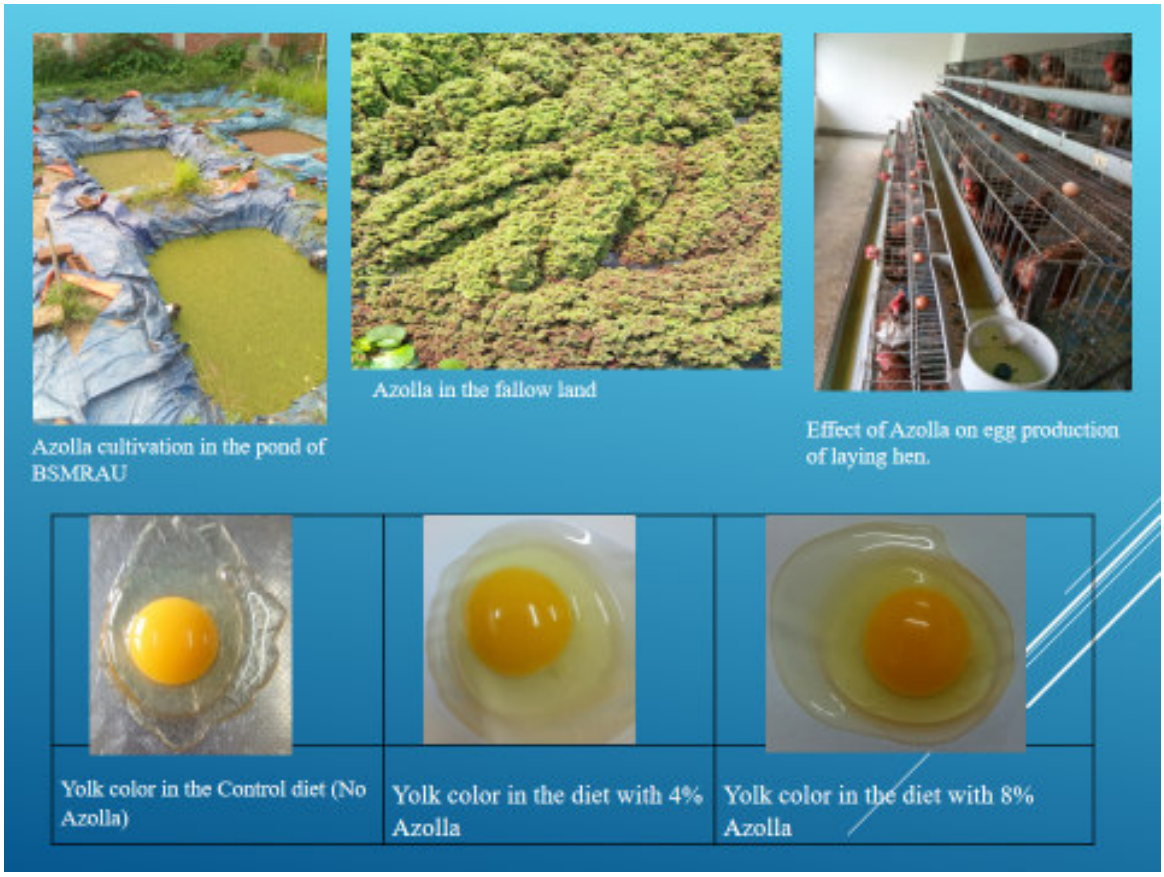

Figure 1. *Azolla* cultivation, and effect of *Azolla* on egg production and yolk color

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC1OC(C[N+](C)(C)C)CC1

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Received: 22 Mar 2020 Revised: 24 Apr 2020 Accepted: 26 May 2020

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona By NC1=CC(=O)NC(=O)N1CC=C

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CCNC(=S)SCCC(=O)O

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by C[N+](C)(C)CC1C[NH]C2CC CCC12

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC(=O)OCCC1SCNC1C

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome".Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6LVN enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identifiedwas CC(=O)OCCC1SCNC1C (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized.

Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [3].

The pharmacophore that was identified had similarity in structure with Gallic acid of Champa plant. The important enzyme of corona virus chosen was 6LVN.

RESULT AND DISCUSSION

Table 1 shows that Gallic acid can block6LVNenzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)OCCC1SCNC1C.

CONCLUSION

The results suggested thatGallic acid can fight againstcorona virus. "Discovery Studio pharmacophoreand Cdockmodule of Biovia software" suggested that the compound capable of deactivating 6LVN enzymehad SMILES valueCC(=O)OCCC1SCNC1C.

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Table 1. Results of C Dock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	CC(=O)OCCC1SCNC1C	10.6805	13.0049

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CCOC(=N)C1CCC(O)CC1

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	CCOC(=N)C1CCC(O)CC1	7.90753	11.9849

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CN1CCCN2CCCN=C12

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RESULT AND DISCUSSION

Table 1 shows that Gallic acid can block6LVNenzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN1CCCN2CCCN=C12.

CONCLUSIONS

The results suggested thatGallic acid can fight againstcorona virus. "Discovery Studio pharmacophoreand Cdockmodule of Biovia software" suggested that the compound capable of deactivating 6LVN enzymehad SMILES valueCN1CCCN2CCCN=C12.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	CN1CCCN2CCCN=C12	6.5941	10.2163

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC1=CC(=O)NC2CC(N)CCC12

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Keywords: Corona, Virus, Docking, Biovia

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	CC1=CC(=O)NC2CC(N)CCC12	2.92419	11.1459

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by O=C1N[C@H](CO1)C2CCCCC2

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC(=O)NC1=NC(=O)NC=C1

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC(C)C[C@H]1S[C@H](C)C(=N1)C

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RESEARCH ARTICLE

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2	Pharmacophore	OC(=O)c1[nH]c(C(=O)O)c2OCCOc12	8.3106	9.96733

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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The pharmacophore that was identified had similarity in structure with Gallic acid of Champa plant. The important enzyme of corona virus chosen was 6LVN.

RESULT AND DISCUSSION

Table 1 shows that Gallic acid can block6LVNenzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1(C)O[C@@H](CC(=O)O)C(=O)O1.

CONCLUSION

The results suggested thatGallic acid can fight againstcorona virus. "Discovery Studio pharmacophoreand Cdockmodule of Biovia software" suggested that the compound capable of deactivating 6LVN enzymehad SMILES valueCC1(C)O[C@@H](CC(=O)O)C(=O)O1.

REFERENCE

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
3. D. Das, S. Das, M. Pandey, D. Bhattacharyay. "In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis", European Journal of Medicinal Plants (2020) 31(4), 19-24.

Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	CC1(C)O[C@@H](CC(=O)O)C(=O)O1	9.23189	7.24652

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RESEARCH ARTICLE

Potassium Ions Affects the Fish Productivity

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ABSTRACT

Here, we aimed to determine the potassium ion of the community based ponds in order to validate the suitability of the pond for aquaculture practices. Potassium ion concentration was measured across three different ponds and finally fish farming was initiated. The potassium was found to be between 1.76 and 7.95 mg-l^{-1}. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Keywords: Community, aquaculture, fish, potassium, ponds.

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60

million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biological characteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi, 2014; Padhi et al. 2015). Mostly, the present study is focused on the determination of quality of water in order to utilize the ponds for aquaculture.

MATERIALS AND METHODS

Site of Study

For the purpose of study, three ponds (P1, P2 and P3) in three villages in the eastern coastal state of India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measurement of Environmental Parameters

The physico-chemical parameter chosen was potassium ion determination. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1).

CONCLUSION

During the period of study, care of the ponds was monitored by a group of peer volunteers from each village who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of fish was being used as seed money by the volunteers for cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

Author Contribution Statement

Sasmita Panda conceived the idea. Pradip Kumar Prusty, Gagan Kumar Panigrahi, Annapurna Sahoo, performed the experiments. Sasmita Panda analyzed the results. All authors contributed significantly in drafting the manuscript.

Funding

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Conflict of Interest

The authors declare that they have no conflict of interest.

REFERENCES

1. Adeniji, H.A. and Ovie, S.I. (1982). Study and appraisal for the water quality of the Ase Oli and Niger Rivers. NIFFER Annual Report, 15-20.
2. APHA. (2005). Standard methods for examination for water and waste water, 17th edition. American Public Health Association. Washington DC.
3. Boyd, C.E. (1989). Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham Ala Aubum University Press.
4. Boyd, C.E. (1990). Water quality in ponds for aquaculture. Albama agricultural experiment station, Auburn University.
5. Das, S.K. and Padhi, S.N. (2014). In Application of Biology for Self Employment. Ed. I Vol. 1, Nanda Kishore Publication, Bhubaneswar, India.
6. Dey, M. M., Rab, M. A., Paraguas, J. P., Piumsombun, S., Bhatta, R., Alam, M. F., & Ahmed, M. (2005). Fish consumption and food security: a disaggregated analysis by types of fish and classes of consumers in selected Asia countries. Aquaculture Economics and Management, 9, 89–111.
7. Dey, M. M., & Prein, M. (2006). Community-based fish culture in seasonal floodplains. Naga, 29(1 & 2), 21–27.
8. EPA, (2006). "Water Quality Standards Review and Revision, Washington DC.
9. Gupta, S.K. and Gupta, P.C. (2006). General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
10. Grafton, R. Q., Williams, J., & Jiang, Q. (2015). Food and water gaps to 2050: preliminary results from the global food and water system (GFWS) platform. Food Security, 7(2), 209–220.
11. Huang, F., Liu, Z., Ridoutt, B. G., Huang, J., & Li, B. (2015). China's water for food under growing water scarcity. Food Security, 7(5), 933–949.
12. Jhingram, V.G. (1985). Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
13. Mahananda, M.R., B.P. Mohanty & N.R. Behera. (2010). Physico-chemical analysis of surface and ground water of Bargarh District, Orissa, India. Int. J. Res. Rev. Appl. Sci., 2(3): 23-29
14. Nagabhatla, N., Beveridge, M., Haque, A. B. M. M., Sophie Nguyen-Khoa, S.,& Brakel, M. V. (2012).Multiple water use as an approach for increased basin productivity and improved adaptation: a case study from Bangladesh. International Journal of River Basin Management, 10(1), 121–136.
15. Nikolosky, G.V. (1963). The ecology of fishes. Academic Press, London, U.K.
16. Olopade, daniyi. (2013). Lakes reservoirs and ponds, 7 (1), 9-19.
17. Padhi, S.N., Das, S.K.,Panda, A. and Panda, Sasmita. (2015). In Employment through aquaculture. Nanda Kishore Publication, Bhubaneswar.
18. Patil, A.A. (2013). Status of water quality of Bhambarde and Lengre reservoir of Sangli district, Maharashtra (India). Flora and Fauna, 19(1): 35-40
19. Philips, M.J., Beveridge, M.C.M. and Clark R.M. (1991). Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture, 3:568-591.
20. Sharma, K., K. Shvetambri, P. Verma & S. P. Sharma. (2009). Physico-chemical assessment of three freshwater ponds of Jammu (J&K), Curr. World Environ, 4(2): 367-373.
21. Zweig, R.D., Morton, J.D. and Stewart, M.M. (1999). Source water quality for aquaculture. A guide for assessment World Bank Report, 74.

Table I: Variations in potassium (mg-l^{-1}) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	2.1	2.98	3.08
Dec-18	2.84	4.1	3.8
Jan-19	3.92	4.92	5.94
Feb-19	3.76	3.98	6.25
Mar-19	4.9	5.98	6.05
Apr-19	5.84	7.2	7.95
May-19	2.37	3.15	6.01
Jun-19	1.76	3.1	3.25
Jul-19	2.17	3.05	3.24
Aug-19	2.59	1.98	2.75
Sep-19	2.08	1.97	2.24
Oct-19	1.95	2.35	2.38
Nov-19	2.08	3.25	3.42

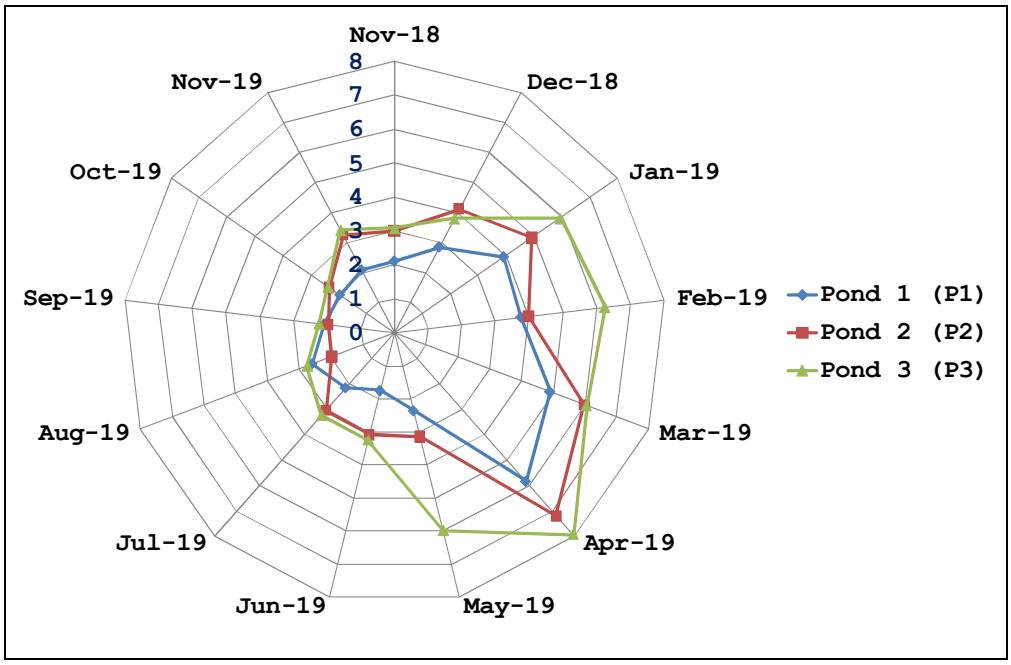

Fig.1: Variations in potassium (mg-l^{-1}) in different ponds in the study area.

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RESEARCH ARTICLE

Fish Productivity is affected by the Concentration of Magnesium Ions

Pradip Kumar Prusty[1], Gagan Kumar Panigrahi[1], Annapurna Sahoo[2] and Sasmita Panda[3]*

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ABSTRACT

Here, we aimed to determine the magnesium ion of the community based ponds in order to validate the suitability of the pond for aquaculture practices. Magnesium ion concentration was measured across three different ponds and finally fish farming was initiated. The magnesium was found to be between 8.87 and 31.84 mg-l^{-1}. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Keywords: Community, aquaculture, fish, magnesium, ponds.

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60

million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biological characteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi, 2014; Padhi et al. 2015). Mostly, the present study is focused on the determination of quality of water in order to utilize the ponds for aquaculture.

MATERIALS AND METHODS

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Measurement of Environmental Parameters

The physico-chemical parameter chosen was magnesium ion determination. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1).

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3. Boyd, C.E. (1989). Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham Ala Aubum University Press.
4. Boyd, C.E. (1990). Water quality in ponds for aquaculture. Albama agricultural experiment station, Auburn University.
5. Das, S.K. and Padhi, S.N. (2014). In Application of Biology for Self Employment. Ed. I Vol. 1, Nanda Kishore Publication, Bhubaneswar, India.
6. Dey, M. M., Rab, M. A., Paraguas, J. P., Piumsombun, S., Bhatta, R., Alam, M. F., & Ahmed, M. (2005). Fish consumption and food security: a disaggregated analysis by types of fish and classes of consumers in selected Asia countries. Aquaculture Economics and Management, 9, 89–111.
7. Dey, M. M., & Prein, M. (2006). Community-based fish culture in seasonal floodplains. Naga, 29(1 & 2), 21–27.
8. EPA, (2006). "Water Quality Standards Review and Revision, Washington DC.
9. Gupta, S.K. and Gupta, P.C. (2006). General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
10. Grafton, R. Q., Williams, J., & Jiang, Q. (2015). Food and water gaps to 2050: preliminary results from the global food and water system (GFWS) platform. Food Security, 7(2), 209–220.
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12. Jhingram, V.G. (1985). Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
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15. Nikolosky, G.V. (1963). The ecology of fishes. Academic Press, London, U.K.
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19. Philips, M.J., Beveridge, M.C.M. and Clark R.M. (1991). Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture, 3:568-591.
20. Sharma, K., K. Shvetambri, P. Verma & S. P. Sharma. (2009). Physico-chemical assessment of three freshwater ponds of Jammu (J&K), Curr. World Environ, 4(2): 367-373.
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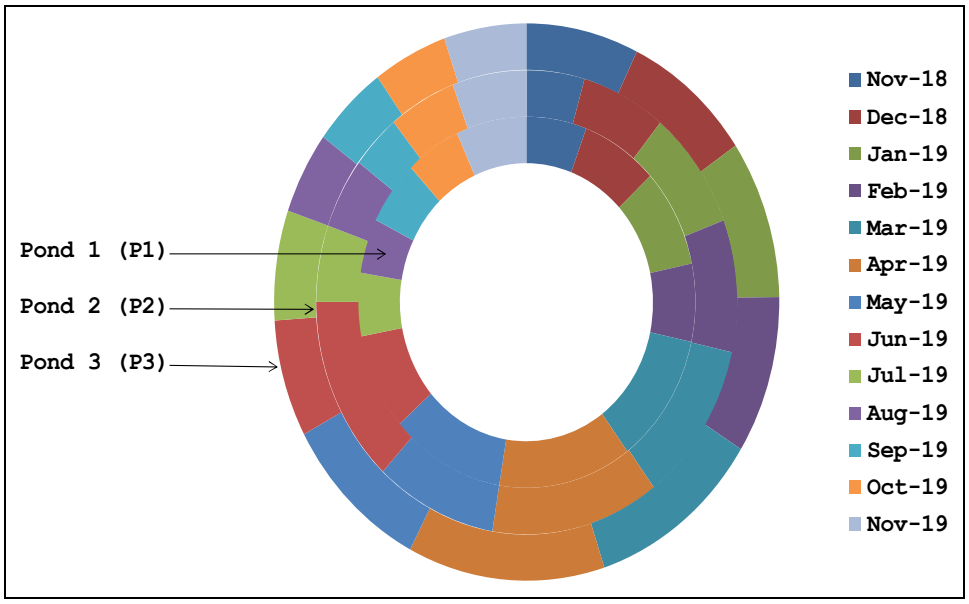
Table I: Variations in magnesium (mg-l^{-1}) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	9.58	9.58	18.2
Dec-18	12.25	14.2	21.1
Jan-19	14.25	18.1	23.33
Feb-19	11.3	20.15	23.25
Mar-19	18.94	24.38	28.34
Apr-19	21.27	28.15	31.84
May-19	18.34	20.39	24.18
Jun-19	14.1	28.3	17.25
Jul-19	9.1	11.6	16.25
Aug-19	7.98	10.75	12.1
Sep-19	9.34	8.35	12.3
Oct-19	8.87	11.25	12.1
Nov-19	11.25	12.45	13.34



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RESEARCH ARTICLE

Calcium Ions may be Critical for Fish Culture

Pradip Kumar Prusty[1], Gagan Kumar Panigrahi[1], Annapurna Sahoo[2] and Sasmita Panda[3]*

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ABSTRACT

Here, we aimed to determine the calcium ion of the community based ponds in order to validate the suitability of the pond for aquaculture practices. Calcium ion concentration was measured across three different ponds and finally fish farming was initiated. The calcium was found to be between 38.12 and 134.4 mg-l^{-1}. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Keywords: Community, aquaculture, fish, calcium, ponds.

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REFERENCES

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2. APHA. (2005). Standard methods for examination for water and waste water, 17th edition. American Public Health Association. Washington DC.
3. Boyd, C.E. (1989). Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham Ala Aubum University Press.
4. Boyd, C.E. (1990). Water quality in ponds for aquaculture. Albama agricultural experiment station, Auburn University.
5. Das, S.K. and Padhi, S.N. (2014). In Application of Biology for Self Employment. Ed. I Vol. 1, Nanda Kishore Publication, Bhubaneswar, India.
6. Dey, M. M., Rab, M. A., Paraguas, J. P., Piumsombun, S., Bhatta, R., Alam, M. F., & Ahmed, M. (2005). Fish consumption and food security: a disaggregated analysis by types of fish and classes of consumers in selected Asia countries. Aquaculture Economics and Management, 9, 89–111.
7. Dey, M. M., & Prein, M. (2006). Community-based fish culture in seasonal floodplains. Naga, 29(1 & 2), 21–27.
8. EPA, (2006). "Water Quality Standards Review and Revision, Washington DC.
9. Gupta, S.K. and Gupta, P.C. (2006). General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
10. Grafton, R. Q., Williams, J., & Jiang, Q. (2015). Food and water gaps to 2050: preliminary results from the global food and water system (GFWS) platform. Food Security, 7(2), 209–220.
11. Huang, F., Liu, Z., Ridoutt, B. G., Huang, J., & Li, B. (2015). China's water for food under growing water scarcity. Food Security, 7(5), 933–949.
12. Jhingram, V.G. (1985). Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
13. Mahananda, M.R., B.P. Mohanty & N.R. Behera. (2010). Physico-chemical analysis of surface and ground water of Bargarh District, Orissa, India. Int. J. Res. Rev. Appl. Sci., 2(3): 23-29
14. Nagabhatla, N., Beveridge, M., Haque, A. B. M. M., Sophie Nguyen-Khoa, S.,& Brakel, M. V. (2012).Multiple water use as an approach for increased basin productivity and improved adaptation: a case study from Bangladesh. International Journal of River Basin Management, 10(1), 121–136.
15. Nikolosky, G.V. (1963). The ecology of fishes. Academic Press, London, U.K.
16. Olopade, daniyi. (2013). Lakes reservoirs and ponds, 7 (1), 9-19.
17. Padhi, S.N., Das, S.K.,Panda, A. and Panda, Sasmita. (2015). In Employment through aquaculture. Nanda Kishore Publication, Bhubaneswar.
18. Patil, A.A. (2013). Status of water quality of Bhambarde and Lengre reservoir of Sangli district, Maharashtra (India). Flora and Fauna, 19(1): 35-40
19. Philips, M.J., Beveridge, M.C.M. and Clark R.M. (1991). Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture, 3:568-591.
20. Sharma, K., K. Shvetambri, P. Verma & S. P. Sharma. (2009). Physico-chemical assessment of three freshwater ponds of Jammu (J&K), Curr. World Environ, 4(2): 367-373.
21. Zweig, R.D., Morton, J.D. and Stewart, M.M. (1999). Source water quality for aquaculture. A guide for assessment World Bank Report, 74.

Table I: Variations in calcium (mg-l^{-1}) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	80.36	82.64	89.1
Dec-18	102.38	103.56	106.3
Jan-19	104.2	110.16	108.12
Feb-19	108.05	112.52	116.5
Mar-19	112.2	120.3	120.1
Apr-19	114.09	127.5	126.8
May-19	120.24	132.5	134.4
Jun-19	64.79	82.45	96.52
Jul-19	47.14	72.5	87.24
Aug-19	38.12	65.2	78.6
Sep-19	48.12	54.2	64.18
Oct-19	50.58	58.45	68.15
Nov-19	62.5	66.5	78.1

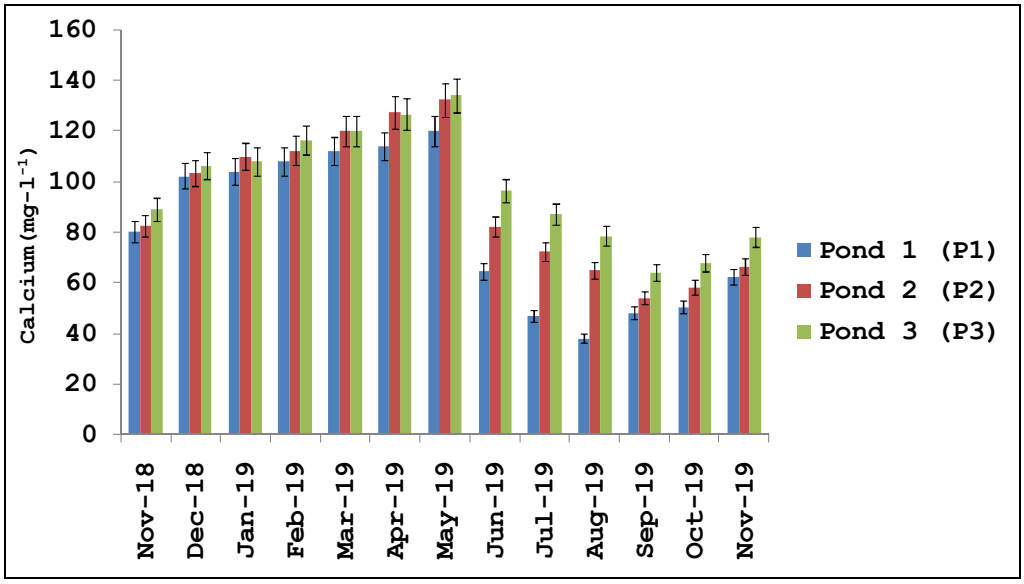

Fig.1: Variations in calcium (mg-l^{-1}) in different ponds in the study area.

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RESEARCH ARTICLE

Fish Productivity is Modulated by the Sodium Ions

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ABSTRACT

Here, we aimed to determine the sodium ion of the community based ponds in order to validate the suitability of the pond for aquaculture practices. Sodium ion concentration was measured across three different ponds and finally fish farming was initiated. The sodiumwas found to be between 9.05 and 27.88 mg-l^{-1}. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Keywords: Community, aquaculture, fish, sodium, ponds.

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60

million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biological characteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi, 2014; Padhi et al. 2015). Mostly, the present study is focused on the determination of quality of water in order to utilize the ponds for aquaculture.

MATERIALS AND METHODS

Site of Study

For the purpose of study, three ponds (P1, P2 and P3) in three villages in the eastern coastal state of India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measurement of Environmental Parameters

The physico-chemical parameter chosen was sodium ion determination. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1).

CONCLUSION

During the period of study, care of the ponds was monitored by a group of peer volunteers from each village who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of fish was being used as seed money by the volunteers for cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

Author Contribution Statement

Sasmita Panda conceived the idea. Pradip Kumar Prusty, Gagan Kumar Panigrahi, Annapurna Sahoo, performed the experiments. Sasmita Panda analyzed the results. All authors contributed significantly in drafting the manuscript.

Funding

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Conflict of Interest

The authors declare that they have no conflict of interest.

REFERENCES

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2. APHA. (2005). Standard methods for examination for water and waste water, 17th edition. American Public Health Association. Washington DC.
3. Boyd, C.E. (1989). Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham Ala Aubum University Press.
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7. Dey, M. M., & Prein, M. (2006). Community-based fish culture in seasonal floodplains. Naga, 29(1 & 2), 21–27.
8. EPA, (2006). "Water Quality Standards Review and Revision, Washington DC.
9. Gupta, S.K. and Gupta, P.C. (2006). General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
10. Grafton, R. Q., Williams, J., & Jiang, Q. (2015). Food and water gaps to 2050: preliminary results from the global food and water system (GFWS) platform. Food Security, 7(2), 209–220.
11. Huang, F., Liu, Z., Ridoutt, B. G., Huang, J., & Li, B. (2015). China's water for food under growing water scarcity. Food Security, 7(5), 933–949.
12. Jhingram, V.G. (1985). Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
13. Mahananda, M.R., B.P. Mohanty & N.R. Behera. (2010). Physico-chemical analysis of surface and ground water of Bargarh District, Orissa, India. Int. J. Res. Rev. Appl. Sci., 2(3): 23-29
14. Nagabhatla, N., Beveridge, M., Haque, A. B. M. M., Sophie Nguyen-Khoa, S.,& Brakel, M. V. (2012).Multiple water use as an approach for increased basin productivity and improved adaptation: a case study from Bangladesh. International Journal of River Basin Management, 10(1), 121–136.
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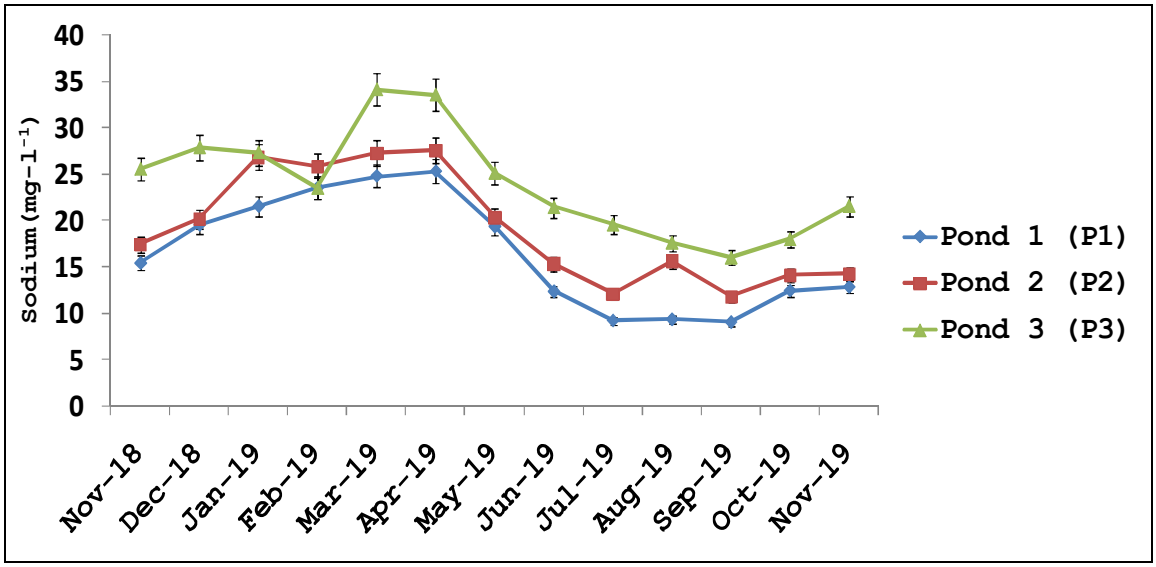
Table I: Variations in sodium (mg-l^{-1}) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	15.42	17.42	25.54
Dec-18	19.53	20.2	27.88
Jan-19	21.55	26.82	27.35
Feb-19	23.56	25.86	23.48
Mar-19	24.81	27.24	34.1
Apr-19	25.32	27.52	33.55
May-19	19.35	20.32	25.1
Jun-19	12.35	15.34	21.42
Jul-19	9.22	12.1	19.56
Aug-19	9.36	15.65	17.6
Sep-19	9.05	11.84	15.98
Oct-19	12.45	14.1	17.96
Nov-19	12.85	14.25	21.56



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RESEARCH ARTICLE

Organic Matter in the Pond Affects the Fish Productivity

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ABSTRACT

Here, we aimed to determine the dissolved organic matter of the ponds so as to make use of the community ponds for aquaculture practices. Dissolved organic matter was measured across three different ponds and finally fish farming was initiated. The dissolved organic matter was found to be between 0.48 and 4.62 mg-l^{-1}. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Keywords: Community, aquaculture, fish, organic matter, ponds.

INTRODUCTION

Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Extensive limnological studies have been carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biological characteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi, 2014; Padhi et al. 2015). Mostly, the present study is focused on the determination of quality of water in order to utilize the ponds for aquaculture.

MATERIALS AND METHODS

Site of Study

For the purpose of study, three ponds (P1, P2 and P3) in three villages in the eastern coastal state of India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measurement of Environmental Parameters

The physico-chemical parameter chosen was specific conductivity. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1).

CONCLUSION

During the period of study, care of the ponds was monitored by a group of peer volunteers from each village who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of fish was being used as seed money by the volunteers for cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

Author Contribution Statement

Sasmita Panda conceived the idea. Pradip Kumar Prusty, Gagan Kumar Panigrahi, Annapurna Sahoo, performed the experiments. Sasmita Panda analyzed the results. All authors contributed significantly in drafting the manuscript.

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REFERENCES

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3. Boyd, C.E. (1989). Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham Ala Aubum University Press.
4. Boyd, C.E. (1990). Water quality in ponds for aquaculture. Albama agricultural experiment station, Auburn University.
5. Das, S.K. and Padhi, S.N. (2014). In Application of Biology for Self Employment. Ed. I Vol. 1, Nanda Kishore Publication, Bhubaneswar, India.
6. Dey, M. M., Rab, M. A., Paraguas, J. P., Piumsombun, S., Bhatta, R., Alam, M. F., & Ahmed, M. (2005). Fish consumption and food security: a disaggregated analysis by types of fish and classes of consumers in selected Asia countries. Aquaculture Economics and Management, 9, 89–111.
7. Dey, M. M., & Prein, M. (2006). Community-based fish culture in seasonal floodplains. Naga, 29(1 & 2), 21–27.
8. EPA, (2006). "Water Quality Standards Review and Revision, Washington DC.
9. Gupta, S.K. and Gupta, P.C. (2006). General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
10. Grafton, R. Q., Williams, J., & Jiang, Q. (2015). Food and water gaps to 2050: preliminary results from the global food and water system (GFWS) platform. Food Security, 7(2), 209–220.
11. Huang, F., Liu, Z., Ridoutt, B. G., Huang, J., & Li, B. (2015). China's water for food under growing water scarcity. Food Security, 7(5), 933–949.
12. Jhingram, V.G. (1985). Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
13. Mahananda, M.R., B.P. Mohanty & N.R. Behera. (2010). Physico-chemical analysis of surface and ground water of Bargarh District, Orissa, India. Int. J. Res. Rev. Appl. Sci., 2(3): 23-29
14. Nagabhatla, N., Beveridge, M., Haque, A. B. M. M., Sophie Nguyen-Khoa, S.,& Brakel, M. V. (2012).Multiple water use as an approach for increased basin productivity and improved adaptation: a case study from Bangladesh. International Journal of River Basin Management, 10(1), 121–136.
15. Nikolosky, G.V. (1963). The ecology of fishes. Academic Press, London, U.K.
16. Olopade, daniyi. (2013). Lakes reservoirs and ponds, 7 (1), 9-19.
17. Padhi, S.N., Das, S.K.,Panda, A. and Panda, Sasmita. (2015). In Employment through aquaculture. Nanda Kishore Publication, Bhubaneswar.
18. Patil, A.A. (2013). Status of water quality of Bhambarde and Lengre reservoir of Sangli district, Maharashtra (India). Flora and Fauna, 19(1): 35-40
19. Philips, M.J., Beveridge, M.C.M. and Clark R.M. (1991). Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture, 3:568-591.
20. Sharma, K., K. Shvetambri, P. Verma & S. P. Sharma. (2009). Physico-chemical assessment of three freshwater ponds of Jammu (J&K), Curr. World Environ, 4(2): 367-373.
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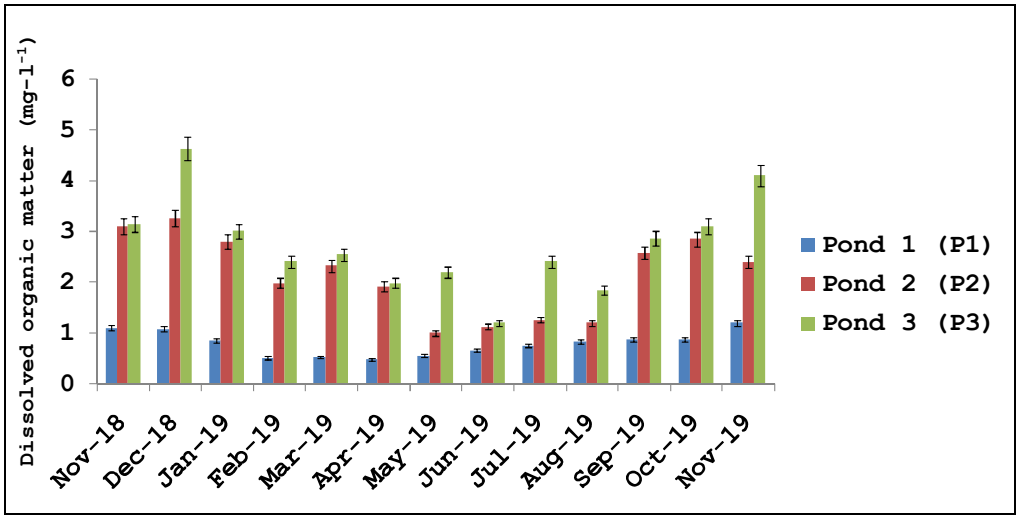
Table I: Variations in dissolved organic matter (mg-l^{-1}) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	1.1	3.1	3.15
Dec-18	1.08	3.26	4.62
Jan-19	0.86	2.8	3
Feb-19	0.51	1.98	2.41
Mar-19	0.52	2.32	2.54
Apr-19	0.48	1.92	1.98
May-19	0.56	1	2.2
Jun-19	0.66	1.12	1.2
Jul-19	0.75	1.26	2.41
Aug-19	0.84	1.2	1.85
Sep-19	0.88	2.58	2.86
Oct-19	0.88	2.85	3.1
Nov-19	1.2	2.4	4.1



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RESEARCH ARTICLE

Fish Productivity is Modulated by the Specific Conductivity of the Pond Water

Pradip Kumar Prusty[1], Gagan Kumar Panigrahi[1], Annapurna Sahoo[2] and Sasmita Panda[3]*

[1]School of Applied Sciences, Centurion University of Technology and Management, Odisha, India.
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ABSTRACT

Here, we aimed to determine the specific conductivity of the community based ponds in order to validate the suitability of the pond for aquaculture practices. Specific conductivity was measured across three different ponds and finally fish farming was initiated. The specific conductivity was found to be between 287 and 660 μs-cm^{-1}. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Keywords: Community, aquaculture, fish, specific conductivity, ponds.

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth

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8. EPA, (2006). "Water Quality Standards Review and Revision, Washington DC.
9. Gupta, S.K. and Gupta, P.C. (2006). General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
10. Grafton, R. Q., Williams, J., & Jiang, Q. (2015). Food and water gaps to 2050: preliminary results from the global food and water system (GFWS) platform. Food Security, 7(2), 209–220.
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12. Jhingram, V.G. (1985). Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
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15. Nikolosky, G.V. (1963). The ecology of fishes. Academic Press, London, U.K.
16. Olopade, daniyi. (2013). Lakes reservoirs and ponds, 7 (1), 9-19.
17. Padhi, S.N., Das, S.K.,Panda, A. and Panda, Sasmita. (2015). In Employment through aquaculture. Nanda Kishore Publication, Bhubaneswar.
18. Patil, A.A. (2013). Status of water quality of Bhambarde and Lengre reservoir of Sangli district, Maharashtra (India). Flora and Fauna, 19(1): 35-40
19. Philips, M.J., Beveridge, M.C.M. and Clark R.M. (1991). Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture, 3:568-591.
20. Sharma, K., K. Shvetambri, P. Verma & S. P. Sharma. (2009). Physico-chemical assessment of three freshwater ponds of Jammu (J&K), Curr. World Environ, 4(2): 367-373.
21. Zweig, R.D., Morton, J.D. and Stewart, M.M. (1999). Source water quality for aquaculture. A guide for assessment World Bank Report, 74.

Table I: Variations in specific conductivity (µs-cm^{-1}) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	327	384	412
Dec-18	287	418	514
Jan-19	351	450	493
Feb-19	327	437	487
Mar-19	430	512	660
Apr-19	412	527	657
May-19	430	521	605
Jun-19	381	501	582
Jul-19	392	387	480
Aug-19	432	458	514
Sep-19	362	411	425
Oct-19	315	362	378

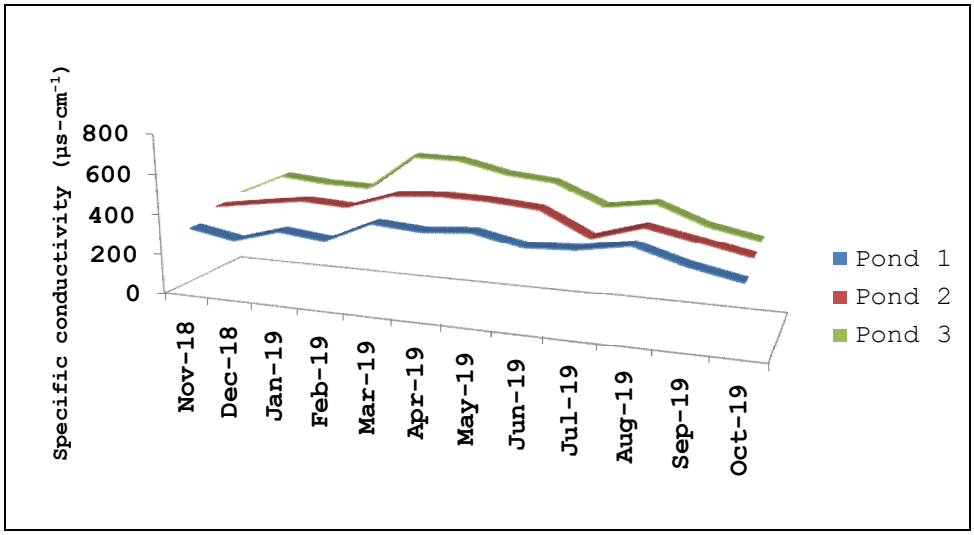

Fig.1: Variations in specific conductivity (µs-cm^{-1}) in different ponds in the study area..

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RESEARCH ARTICLE

Alkalinity of the Pond Water Contributes to Fish Productivity

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ABSTRACT

Aquaculture being the fastest growing food production sector, we focused on community-based pond aquaculture on the eastern coastal regions of India. Essentially, we aimed to determine the alkalinity of the community based ponds in order to validate the suitability of the pond for aquaculture practices. Alkalinity was measured across three different ponds and finally fish farming was initiated. The alkalinity was found to be between 82.347 and 198.346 mg $CaCO_3$-l^{-1}. Essentially, this diagnostic approach demonstrates how sustainability challenges can be countered at the community level. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy.

Keywords: Community, aquaculture, fish, alkalinity, ponds

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic

ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60 million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biological characteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi, 2014; Padhi et al. 2015). Mostly, the present study is focused on the determination of quality of water in order to utilize the ponds for aquaculture. The Main objectives of the study was to determine physical, chemical and biological characteristics of ponds in order to utilize them for fish culture and thus generate employment opportunity for gainful earning among rural people by creating awareness among them through training on aquaculture practices. Composite fish farming is the technique to culture different types of compatible and non competitive fishes in the same ecosystem so as to allow them to grow by feeding by making optimum use of different zones (surface, bottom and column) of the ponds without impeding the growth, development and maturity of one another. This is a very profitable method of aquaculture and hence importance has been laid to train the populace for gainful employment.

MATERIALS AND METHODS

Site of Study

For the purpose of study, three ponds (P1, P2 and P3) in three villages in the eastern coastal state of India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measurement of Environmental Parameters

The physico-chemical parameter chosen was alkalinity. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1).

CONCLUSION

During the period of study, care of the ponds was monitored by a group of peer volunteers from each village who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of fish was being used as seed money by the volunteers for cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

Author Contribution Statement

Sasmita Panda and Surendra Nath Padhi conceived the idea. Pradip Kumar Prusty, Gagan Kumar Panigrahi, Annapurna Sahoo, Shraban Kumar Sahoo performed the experiments. Sasmita Panda and Surendra Nath Padhi analyzed the results. All authors contributed significantly in drafting the manuscript.

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Conflict of Interest
The authors declare that they have no conflict of interest.

REFERENCES

1. Adeniji, H.A. and Ovie, S.I. (1982). Study and appraisal for the water quality of the Ase Oli and Niger Rivers. NIFFER Annual Report, 15-20.
2. APHA. (2005). Standard methods for examination for water and waste water, 17th edition. American Public Health Association. Washington DC.
3. Boyd, C.E. (1989). Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham Ala Aubum University Press.
4. Boyd, C.E. (1990). Water quality in ponds for aquaculture. Albama agricultural experiment station, Auburn University.
5. Das, S.K. and Padhi, S.N. (2014). In Application of Biology for Self Employment. Ed. I Vol. 1, Nanda Kishore Publication, Bhubaneswar, India.
6. Dey, M. M., Rab, M. A., Paraguas, J. P., Piumsombun, S., Bhatta, R., Alam, M. F., & Ahmed, M. (2005). Fish consumption and food security: a disaggregated analysis by types of fish and classes of consumers in selected Asia countries. Aquaculture Economics and Management, 9, 89–111.
7. Dey, M. M., & Prein, M. (2006). Community-based fish culture in seasonal floodplains. Naga, 29(1 & 2), 21–27.
8. EPA, (2006). "Water Quality Standards Review and Revision, Washington DC.
9. Gupta, S.K. and Gupta, P.C. (2006). General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
10. Grafton, R. Q., Williams, J., & Jiang, Q. (2015). Food and water gaps to 2050: preliminary results from the global food and water system (GFWS) platform. Food Security, 7(2), 209–220.
11. Huang, F., Liu, Z., Ridoutt, B. G., Huang, J., & Li, B. (2015). China's water for food under growing water scarcity. Food Security, 7(5), 933–949.
12. Jhingram, V.G. (1985). Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
13. Mahananda, M.R., B.P. Mohanty & N.R. Behera. (2010). Physico-chemical analysis of surface and ground water of Bargarh District, Orissa, India. Int. J. Res. Rev. Appl. Sci., 2(3): 23-29
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15. Nikolosky, G.V. (1963). The ecology of fishes. Academic Press, London, U.K.
16. Olopade, daniyi. (2013). Lakes reservoirs and ponds, 7 (1), 9-19.
17. Padhi, S.N., Das, S.K.,Panda, A. and Panda, Sasmita. (2015). In Employment through aquaculture. Nanda Kishore Publication, Bhubaneswar.
18. Patil, A.A. (2013). Status of water quality of Bhambarde and Lengre reservoir of Sangli district, Maharashtra (India). Flora and Fauna, 19(1): 35-40

19. Philips, M.J., Beveridge, M.C.M. and Clark R.M. (1991). Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture, 3:568-591.
20. Sharma, K., K. Shvetambri, P. Verma & S. P. Sharma. (2009). Physico-chemical assessment of three freshwater ponds of Jammu (J&K), Curr. World Environ, 4(2): 367-373.
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Table I: Variations in total alkalinity (mg $CaCO_3$-l^{-1}) in different ponds in the study area.

Month-Year	Pond 1 (P1)	Pond 2 (P2)	Pond 3 (P3)
Nov-18	111.054	100.347	114.287
Dec-18	121.348	154.4	130.274
Jan-19	128.475	137.64	133.258
Feb-19	135.345	154.39	139.647
Mar-19	155.48	163.345	167.854
Apr-19	158.647	193.348	198.346
May-19	89.345	183.328	178.125
Jun-19	84.39	113.347	107.46
Jul-19	82.347	87.396	85.349
Aug-19	96.319	108.394	125.647
Sep-19	84.205	97.321	95.364
Oct-19	97.228	89.367	97.34

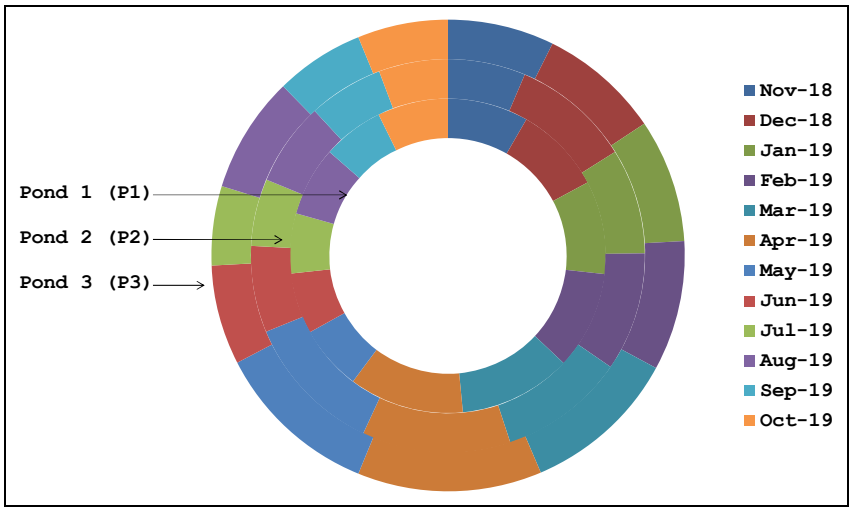

Fig.1: Variations in total alkalinity (mg $CaCO_3$-l^{-1}) in different ponds in the study area

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RESEARCH ARTICLE

Physical Parameters Like Rainfall, Temperature and Relative Humidity Affects the Productivity of a Pond

Pradip Kumar Prusty[1], Gagan Kumar Panigrahi[1], Annapurna Sahoo[2], Shraban Kumar Sahoo[1], Surendra Nath Padhi[3] and Sasmita Panda[4]*

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ABSTRACT

Essentially, in an ecosystem, ecology is considered to be the primary unit of ecology. It provides information concerning the utilization and recycling of mineral elements and the availability of solar energy. Mostly, the living organisms present in an ecosystem contribute to the biotic component while the nonliving factors including the physical and chemical factors constitute the abiotic components of an ecosystem. Essentially, this diagnostic approach demonstrates how sustainability challenges can be countered at the community level. Mostly, we emphasized the need for augmented knowledge and hands on training on effective aquaculture practice.

Keywords: Community, aquaculture, fish, alkalinity, ponds

INTRODUCTION

With an ever increasing food demand, contribution of fish farming is significant. This study primarily focuses on making use of unexploited ponds present in the community aiming for introducing fish farming, resulting in an increment in the local economy. Aquaculture being the fastest growing food production sector, we focused on community-based pond aquaculture on the eastern coastal of India. Water is considered to be a vital natural resource and a critical agricultural input (Huang et al., 2015). Water usage is essential for sustainable agricultural escalation and boost of food availability (Grafton et al., 2015). However, strategies for increasing agricultural productivity need to be focussed. Culture of fish, particularly composite fish culture can be an imperative tool for sustainably

recuperating agricultural productivity and for strengthening rural economies (Nagabhatla et al. 2012; Dey and Prein 2006; Dey et al., 2005). Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009). Limnology essentially deals with inland aquatic ecosystems. Primarily, the growth and survival of fresh water inhabitants depend on the quality of water (Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60 million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biological characteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi, 2014; Padhi et al. 2015). Mostly, the present study is focused on the determination of quality of water in order to utilize the ponds for aquaculture. The Main objectives of the study was to determine physical, chemical and biological characteristics of ponds in order to utilize them for fish culture and thus generate employment opportunity for gainful earning among rural people by creating awareness among them through training on aquaculture practices. Composite fish farming is the technique to culture different types of compatible and non competitive fishes in the same ecosystem so as to allow them to grow by feeding by making optimum use of different zones (surface, bottom and column) of the ponds without impeding the growth, development and maturity of one another. This is a very profitable method of aquaculture and hence importance has been laid to train the populace for gainful employment.

MATERIALS AND METHODS

Site of Study

For the purpose of study, three ponds (P1, P2 and P3) in three villages in the eastern coastal state of India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measurement of Environmental Parameters

The parameters chosen were rainfall, relative humidity and temperature. Measurement was primarily made by following standard procedures (APHA-2005) using water testing kits (NICE), during the period from November 2018 to October 2019.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999). Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment (Table 1 and Fig.1)

CONCLUSION

Awareness programmes were organized periodically in the villages in order to create awareness among people to motivate them for fish cultivation. Training programmes on composite fish farming were organized for villagers and students. The technical expertise so gained is believed to be utilized by the beneficiaries for gainful earning. During the period of study care of the ponds was monitored by a group of peer volunteers from each village who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of

fish was being used as seed money by the volunteers for cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

Author Contribution Statement

Sasmita Panda and Surendra Nath Padhi conceived the idea. Pradip Kumar Prusty, Gagan Kumar Panigrahi, Annapurna Sahoo, Shraban Kumar Sahoo performed the experiments. Sasmita Panda and Surendra Nath Padhi analyzed the results. All authors contributed significantly in drafting the manuscript.

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REFERENCES

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2. APHA. (2005). Standard methods for examination for water and waste water, 17th edition. American Public Health Association. Washington DC.
3. Boyd, C.E. (1989). Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham Ala Aubum University Press.
4. Boyd, C.E. (1990). Water quality in ponds for aquaculture. Albama agricultural experiment station, Auburn University.
5. Das, S.K. and Padhi, S.N. (2014). In Application of Biology for Self Employment. Ed. I Vol. 1, Nanda Kishore Publication, Bhubaneswar, India.
6. Dey, M. M., Rab, M. A., Paraguas, J. P., Piumsombun, S., Bhatta, R., Alam, M. F., & Ahmed, M. (2005). Fish consumption and food security: a disaggregated analysis by types of fish and classes of consumers in selected Asia countries. Aquaculture Economics and Management, 9, 89–111.
7. Dey, M. M., & Prein, M. (2006). Community-based fish culture in seasonal floodplains. Naga, 29(1 & 2), 21–27.
8. EPA, (2006). "Water Quality Standards Review and Revision, Washington DC.
9. Gupta, S.K. and Gupta, P.C. (2006). General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
10. Grafton, R. Q., Williams, J., & Jiang, Q. (2015). Food and water gaps to 2050: preliminary results from the global food and water system (GFWS) platform. Food Security, 7(2), 209–220.
11. Huang, F., Liu, Z., Ridoutt, B. G., Huang, J., & Li, B. (2015). China's water for food under growing water scarcity. Food Security, 7(5), 933–949.
12. Jhingram, V.G. (1985). Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
13. Mahananda, M.R., B.P. Mohanty & N.R. Behera. (2010). Physico-chemical analysis of surface and ground water of Bargarh District, Orissa, India. Int. J. Res. Rev. Appl. Sci., 2(3): 23-29

14. Nagabhatla, N., Beveridge, M., Haque, A. B. M. M., Sophie Nguyen-Khoa, S.,& Brakel, M. V. (2012).Multiple water use as an approach for increased basin productivity and improved adaptation: a case study from Bangladesh. International Journal of River Basin Management, 10(1), 121–136.
15. Nikolosky, G.V. (1963). The ecology of fishes. Academic Press, London, U.K.
16. Olopade, daniyi. (2013). Lakes reservoirs and ponds, 7 (1), 9-19.
17. Padhi, S.N., Das, S.K.,Panda, A. and Panda, Sasmita. (2015). In Employment through aquaculture. Nanda Kishore Publication, Bhubaneswar.
18. Patil, A.A. (2013). Status of water quality of Bhambarde and Lengre reservoir of Sangli district, Maharashtra (India). Flora and Fauna, 19(1): 35-40
19. Philips, M.J., Beveridge, M.C.M. and Clark R.M. (1991). Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture, 3:568-591.
20. Sharma, K., K. Shvetambri, P. Verma & S. P. Sharma. (2009). Physico-chemical assessment of three freshwater ponds of Jammu (J&K), Curr. World Environ, 4(2): 367-373.
21. Zweig, R.D., Morton, J.D. and Stewart, M.M. (1999). Source water quality for aquaculture. A guide for assessment World Bank Report, 74.

Table I: Variations in average rainfall (mm) relative humidity (%) atmospheric temperature (^{0}C) in the study area.

Month-Year	Rainfall	Relative humidity	Minimum atmospheric temperature	Maximum atmospheric temperature
Nov-18	103.61	78	21	28
Dec-18	4.5	80	16.8	27
Jan-19	5.7	84	17.9	28
Feb-19	11.69	75	19	32
Mar-19	5.1	75	24	31
Apr-19	27.3	73	26	35
May-19	18.69	77	28	36
Jun-19	210.37	83	27	34
Jul-19	110.32	79	26.5	32
Aug-19	336.67	87	25.9	32
Sep-19	161.34	83	26.2	31
Oct-19	306.37	87	25.3	30

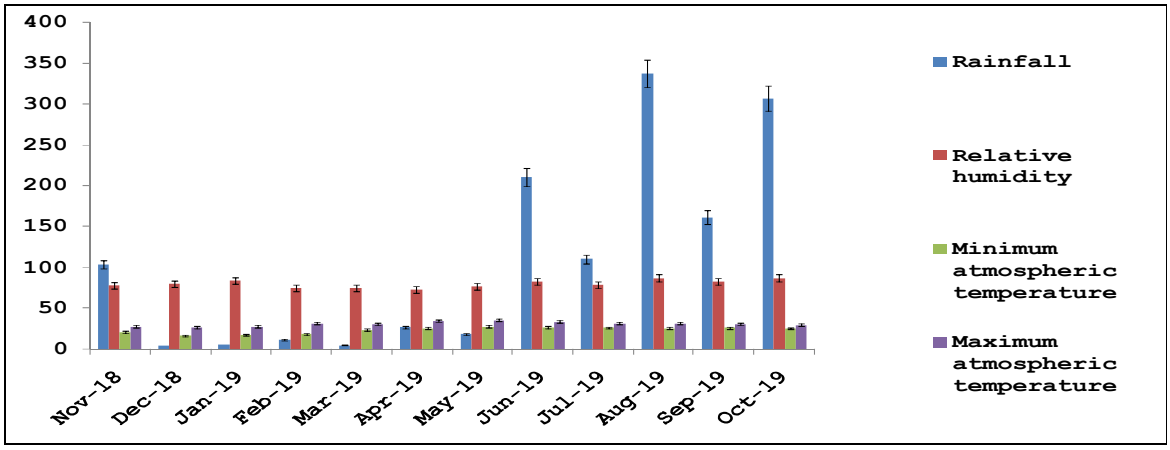

Fig.1: Variations in average rainfall (mm) relative humidity (%) atmospheric temperature (^{0}C) in the study area.

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RESEARCH ARTICLE

Bacteria as a Source of Natural Dye

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ABSTRACT

Numerous pigments have been isolated from a variety of microorganisms including fungi and protozoa. Bacterial pigments are water soluble or insoluble; water soluble pigments are diffused in the growth medium. Chemically, bacterial pigments are pyrrole, phenazine, carotenoid, xanthophylls and quinine or quinone derivatives. Structural information on many of these compounds like quinone which are amphiphilic in nature is an indicative of a strong membrane association potential. So as Food colorants may be classified into synthetic, nature-identical, inorganic, and natural colorants. Most often, the colorants are extracted from plant material, but other sources such as insects, algae, cyanobacteria, and fungi are used as well. A Halophylic bacterium has also been reported of producing different pigments. Synthesis of polymeric pigments is also been extensively studied now a days. The molecular genetic studies of pigment synthesis present vital scope for scaling up industrial importance of useful pigmented bacteria. The main objective of this study is to use pigments from locally isolated coloured bacteria as natural dyes to replace the existing synthetic dye.

Keywords: Carotenoid, colorants, dye, pigment, Gram-positive bacteria, Gram-negative bacteria.

INTRODUCTION

A pigment is a material that changes the color of reflected or transmitted light as the result of wavelength-selective absorption. This physical process differs from fluorescence, phosphorescence, and other forms of luminescence, in which a material emits light. Pigments are used for coloring paint, ink, plastic, fabric, cosmetics, food and other

materials. The worldwide market for inorganic, organic and special pigments had a total volume of around 7.4 million tons in 2006. For this various necessary of pigment they are formed by different chemical methods. But the synthetic dyes have toxic or carcinogenic effects. So to eradicate this problem we must use natural dyes which are produced large amount from different microorganisms. Natural dyes/colorants derived from flora and fauna are believed to be safe because of non-toxic, non-carcinogenic and biodegradable in nature. As the present trend throughout the world is shifting towards the use of eco-friendly and biodegradable commodities, the demand for natural dyes is increasing day by day. Amongst the source of natural pigments are ores, insects, plants and microorganisms. Lately, the potential of using microbial pigments as natural colourants is being investigated. Microbes such as bacteria are one of the most likely sources of new pigments because they have the potential of being exploited using existing culture techniques. The pigments of higher organisms, animal, plant and fungal, may be less accessible to exploitation because of the structural complexity of the pigment-bearing tissue or because the pigment is formed only at critical points of development within a complex life cycle. The natural pigment has various significance. Pigments confer antibacterial and heavy metal resistance. Carotenoids protect pigmented cells against ultraviolet radiation, and therefore many pigmented microorganisms inhabit the air; in photoautotrophic bacteria, carotenoids take part in photosynthesis. Some pigments possess antibiotic properties. The main purpose of this is to use the natural pigment instead of synthetic dyes. Here, we have given a brief overlook on the pigment forming microorganisms like *Rhodospirillum rubrum*, *Chromobacterium violaceum*, *Chlorobium tepidum*.

Pigment Forming Microorganisms

There are different types of microorganisms which can produce the pigments. Mainly the bacteria, fungi & algae produced the coloured pigments. By this process we can got the natural colours and dyes which is more preferable instead the synthetic dye or pigments. Natural pigments are highly resistant to the effects of light and air.

Pigment Forming Bacteria

Bacteria are pigmented or colored. Pigmented bacteria are also known as chromo bacteria. Bacterial pigments are water soluble or insoluble; water soluble pigments are diffused in the growth medium. Chemically, bacterial pigments are pyrrole, phenazine, carotenoid, xanthophylls and quinine or quinone derivatives. The pigment molecules are synthesized in cell wall or periplasmic space. We can visualize pigmentation in bacteria in specific growth medium or by staining bacterial cells with a dye to observe under microscope. It has been proved that only aerobic and facultatively aerobic bacteria are pigmented because, molecular oxygen is essential for pigmentation. Therefore, anaerobic bacteria are nonpigmented. Pigment synthesis is also dependent on light, pH, temperature and media constituents like indicator dyes. They display all the colours from rainbow including light or dark tinges and unusual colours like black, white, brown, golden, silver and fluorescent green, yellow or blue.

Rhodospirillum rubrum

Scientific ClassificationKINGDOM: Bacteria, PHYLUM: Proteobacteria, CLASS: Alpha proteobacteria, ORDER: Rhodospirillales, FAMILY: Rhodospirillaceae, GENUS: *Rhodospirilum*, SPECIES:*rubrum*

Rhodospirillum rubrum (*R. rubrum*) is a Gram-negative, purple-coloured Proteobacterium, with a size of 800 to 1000 nanometres. It is a facultative anaerobe; it can therefore use alcoholic fermentation under low oxygen conditions or use aerobic respiration in aerobic conditions. Under aerobic growth photosynthesis is genetically suppressed and *R. rubrum* is then colourless (Fig.1). After the exhaustion of oxygen, *R. rubrum* immediately starts the production of photosynthesis apparatus including membrane proteins, bacteriochlorophylls and carotenoids, i.e. the bacterium becomes photosynthesis active. *R. rubrum* is also a nitrogen fixing bacterium, i.e., it can express and regulate nitrogenase, a protein complex that can catalyse the conversion of atmospheric dinitrogen into ammonia Selao TT & Nordlund, (2008). Due to this important property, *R. rubrum* has been the test subject of many different groups, so as to understand the complex regulatory schemes required for this reaction to occur Wolfe *et al*., (2007). It was in *R.*

rubrum that, for the first time, post-translational regulation of nitrogenase was demonstrated. Nitrogenase is modified by an ADP-ribosylation in the arginine residue 101 Pope *et al*., (1985) in response to the so-called "switch-off" effectors - glutamine or ammonia - and darkness Neilson and Nordlund, (1975).

R. rubrum has several potential uses in biotechnology:

- Quantitative accumulation of PHB (poly-hydroxy-butric-acid) precursors in the cell for the production of biological plastic
- Production of biological hydrogen fuel
- Model system for studying the conversion from light energy to chemical energy and regulatory pathways of the nitrogen fixation system

Chromobacterium violaceu

Scientific Classification

KINGDOM: Bacteria, PHYLUM: Proteobacteria, CLASS: Betaproteobacteria, ORDER: Neisseriales, FAMILY: Neisseriaceae, GENUS: *Chromobacterium*, SPECIES: *violaceum*

Chromobacterium violaceum is a Gram-negative, facultative anaerobic, non-sporing coccobacillus. It is part of the normal flora of water and soil of tropical and sub-tropical regions of the world (Fig.2). It produces a natural antibiotic called **violacein**, which may be useful for the treatment of colon and other cancers Kodach *et al*., (2006). It grows readily on nutrient agar, producing distinctive smooth low convex colonies with a dark violet metallic sheen (due to violacein production). Its full genome was published in 2003(Brazilian National Genome Project Consortium 2003). It has the ability to break down tarballs Itah *et al*., (2005). Violacein is a violet pigment extracted from the gram-negative bacterium *Chromobacterium violaceum*. It presents bactericidal, tumoricidal, trypanocidal, and antileishmanial activities.

C. violaceum produces a number of natural antibiotics:

- Aztreonam is a monobactam antibiotic that is active against gram-negative aerobic bacteria including *Pseudomonas aeruginosa*. It is marketed as **Azactam**.
- Violacein is active against amoebae and trypanosomes;
- Aerocyanidine is active against Gram-positive organisms;
- Aerocavin is active against Gram-positive and Gram-negative organisms.

Chlorobium tepidum

Scientific Classification

KINGDOM: Bacteria, PHYLUM: Chlorobi, CLASS: Chlorobia, ORDER: Chlorobiales, FAMILY: Chlorobiaceae, GENUS: *Chlorobaculum*, SPECIES: *tepidum*

Chlorobium species exhibit a dark green color; in a Winogradsky column, the green layer often observed is composed of *Chlorobium.* This genus lives in strictly anaerobic conditions below the surface of a body of water, commonly the anaerobic zone of a eutrophic lake Prescott *et al*., (2005). *Chlorobium aggregatum* is a species which exists in a symbiotic relationship with colorless, nonphotosynthetic bacteria (Fig.3). This species looks like a bundle of green bacteria, attached to a central rod-like cell which can move around with a flagellum. The green, outer bacteria use light to oxidize sulfide into sulfate. The inner cell, which is not able to perform photosynthesis, reduces the sulfate into sulfide. These bacteria divide in unison, giving the structure a multicellular appearance which is highly unusual in bacteria Postgate and John, (1994).Chlorosomes are the main light harvesting complexes of green

photosynthetic bacteria. The complete *C. tepidum* genome, which consists of 2.15 megabases (Mb), was sequenced and published in 2002 Eisen *et al.*, (2002). It synthesizes chlorophyll *a* and bacteriochlorophylls (BChls) *a* and *c*, of which the model organism has been used to elucidate the biosynthesis of BChl *c* (Frigaard *etal.* 2006). Several of its carotenoid metabolic pathways (including a novel lycopene cyclase) have similar counterparts in cyanobacteria Frigaard *et al.*, (2004).This suggests that the lamellar model is universal among green sulfur bacteria. In contrast to green-colored *Chl. tepidum*, chlorosomes from the brown-colored species often contain domains of lamellar aggregates that may help them to survive in extremely low light conditions. We suggest that carotenoids are localized between the lamellar planes and drive lamellar assembly by augmenting hydrophobic interactions

CONCLUSION

Pigments confer antibacterial and heavy metal resistance. Pathogenic staphylococci are multidrug resistant because of their pigment which acts as barrier for antibiotics acting on cell wall and plasma membrane. Bacteria showing heavy metal resistance are usually pigmented as they have been exploited for remediation of soil and water polluted by heavy metals like arsenic, copper, cadmium, mercury and nickel. Pigmented bacteria have also been used as biosensors to detect environmental pollution like oil spills or pesticide and heavy metal recalcitrance. Pigments are important characteristics of particular genus and are very helpful in the identification and classification of microorganisms. The best example of pigmentation is Xanthomonas spp. All the species of Xanthomonas produce yellow colored pigments known as xanthomonadins. Taxonomically, xanthomonadin synthesis is an important trait because they have similar chromatographic and absorption spectra which form the basis of classification of xanthomonads. The molecular genetic studies of pigment synthesis present vital scope for scaling up industrial importance of useful pigmented bacteria.

Author Contribution Statement

Annapurna Sahoo and Gagan Kumar Panigrahi conceived the idea. All authors contributed significantly in drafting the manuscript.

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Conflict of Interest

The authors declare that they have no conflict of interest.

REFERENCES

1. Itah A. Y., Essien J. P. "Growth Profile and Hydrocarbonoclastic Potential of Microorganisms Isolated from Tarballs in the Bight of Bonny, Nigeria". *World Journal of Microbiology and Biotechnology* (2005): 21: 1317–1322. Print.
2. J.A. Eisen; Nelson, KE; Paulsen, IT; Heidelberg, JF; Wu, M; Dodson, RJ; Deboy, R; Gwinn, ML et al. "The complete genome sequence of the green sulfur bacterium *Chlorobium tepidum*". *Proc. Natl Acad. Sci. USA* (2002): 99 (14): 9509–9514. Print.
3. Kodach LL, Bos CL, Durán N, Peppelenbosch MP, Ferreira CV, Hardwick JC. "Violacein synergistically increases 5-fluorouracil cytotoxicity, induces apoptosis and inhibits Akt-mediated signal transduction in human colorectal cancer cells". *Carcinogenesis* (2006): 27 (3): 508–16. Print.

4. N.-U. Frigaard, *et al*. "Genetic manipulation of carotenoid biosynthesis in the green sulfur bacterium *Chlorobium tepidum*". *Proc. Natl Acad. Sci. USA* (2004): 186: 5210–5220.Print.
5. Neilson AH, Nordlund S. "Regulation of nitrogenase synthesis in intact cells of Rhodospirillum rubrum: inactivation of nitrogen fixation by ammonia, L-glutamine and L-asparagine". *J Gen Microbiol* (1975): 91 (1): 53–62. Print.
6. Pope MR, Murrell SA, Ludden PW. "Covalent modification of the iron protein of nitrogenase from Rhodospirillum rubrum by adenosine diphosphoribosylation of a specific arginine residue". *Proc Nate Cad Sci U S A* (1985): 82 (10): 3173–7. Print.
7. Postgate, John: "The Outer Reaches of Life". Cambridge University Press (1994): 132-134. Print.
8. Prescott, Harley, Klein. *Microbiology* pp. (2005): 195, 493, 597, 618-619, 339. Print.
9. Selao TT, Nordlund S, Norén A. "Comparative proteomic studies in *Rhodospirillum rubrum* grown under different nitrogen conditions". *J Proteome Res* (2008): 7 (8): 3267–75. Print.
10. Wolfe DM, Zhang Y, and Roberts GP. "Specificity and Regulation of Interaction between the PII and AmtB1 Proteins in *Rhodospirillum rubrum*". *J Bacteriol* (2007): 189 (19): 6861–6869. Print.

Table. 1. Pigment forming microorganisms

Purple	*Spirillium rubum*
Violet	*Chrombacterium violacein*
Indigo	*Janthinobacterium violacein*
Blue	*Streptomyces coelicolor*
Green	*Chlorobium tepidum*
Yellow	*Xanthomonas campestris*
Orange	*Sarcina aurentiaca*
Red	*Serratia marcescens*
Brown	*Rhizobium etli*
Black	*Prevotela melaninogenica*
Golden	*Staphylococcus aureus*
Silver	*Actinomyces sp*
White	*Staphylococcus epidermidis*
Cream	*Proteus vulgaris*
Pink	*Micrococcus roseus*
Maroon	*Rugamonas rubra*
Fluorescent blue/green	*Pseudomonas aeruginosa*

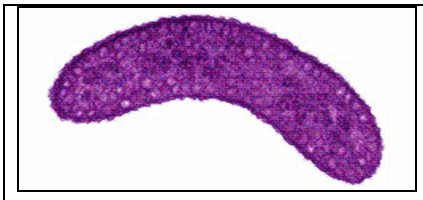

Fig.1 *Rhodospirillum rubru*

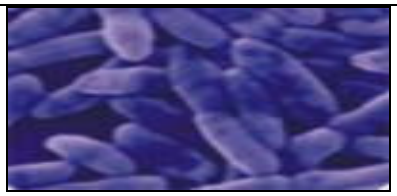

Fig.2 *Chromobacterium violaceum*

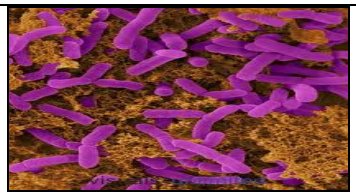

Fig.3 *Chlorobium tepidum*

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RESEARCH ARTICLE

Ebola, a Viral Hemorrhagic Fever of Humans and other Primates

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ABSTRACT

Ebola virus disease (EVD) or Ebola hemorrhagic fever (EHF) is a viral hemorrhagic fever, often fatal illness in humans and nonhuman primates (monkeys, gorillas, and chimpanzees) caused by ebola viruses. EVD have a case fatality rate of up to 90%. Ebola viruses are found in several African countries. First in 1976, Ebola appeared in two simultaneous outbreaks, in Nzara, Sudan, and in Yambuku, Democratic Republic of Congo. The latter was in a village situated near the Ebola River, from which the disease takes its name. Since then, outbreaks have appeared sporadically in Africa. However, on the basis of evidence and the nature of similar viruses, researchers believe that the virus is animal-borne and that bats are the most likely reservoir. Four of the five subtypes of ebola virus occur in an animal host native to Africa. The risk to human health is likely to be low for healthy adults but is unknown for all other population groups.

Keywords: Ebola Virus, Ebola hemorrhagic fever, Primates , human health

INTRODUCTION

Ebola virus disease (EVD) or Ebola hemorrhagic fever (EHF) is a viral hemorrhagic fever, often fatal illness in humans and nonhuman primates (monkeys, gorillas, and chimpanzees) caused by ebola viruses. EVD have a case fatality rate of up to 90%. Ebola viruses are found in several African countries. First in 1976, Ebola appeared in two simultaneous outbreaks, in Nzara, Sudan, and in Yambuku, Democratic Republic of Congo. The latter was in a

village situated near the Ebola River, from which the disease takes its name. Since then, outbreaks have appeared sporadically in Africa. However, on the basis of evidence and the nature of similar viruses, researchers believe that the virus is animal-borne and that bats are the most likely reservoir. Four of the five subtypes of ebola virus occur in an animal host native to Africa. The risk to human health is likely to be low for healthy adults but is unknown for all other population groups.

Cause and Agent

Ebolavirus belongs to the Filoviridae family (filovirus), genus Ebolavirus. Ebolavirus comprises 5 distinct species:
1. Bundibugyo ebolavirus (BDBV)
2. Zaire ebolavirus (EBOV)
3. Sudan ebolavirus (SUDV)
4. Reston ebolavirus (RESTV)
5. Taï Forest ebolavirus (TAFV)

Four of the five have caused disease in humans: Ebola virus (Zaire ebolavirus); Sudan virus (Sudan ebolavirus); Taï Forest virus (Taï Forest ebolavirus, formerly Côte d'Ivoire ebolavirus); and Bundibugyo virus (Bundibugyo ebolavirus). Pathogenicity varies among Ebola viruses, from EBOV, which ishighly lethal in humans, to RESTV, which causes disease in pigs and macaques butasymptomatically infects humans. TheRESTV is not as great a threat as the other ebolaviruses that are known to be highly pathogenic for humans. The natural reservoir host of Ebola viruses remains unknown.

Disease Agent Characteristics

a) Virion Morphology and Size: Enveloped, helical,cross-striated nucleo capsid, filamentous or pleomor-phic virions that are flexible with extensive branch-ing, 80 nm in diameter and 970-1200 nm in length.
b)Nucleic Acid: Linear, negative-sense, single-stranded RNA, ~18,900 kb in length.
c) Physicochemical Properties: Stable at room temperature and can resist desiccation; inactivated at 60°C for30 minutes; infectivity greatly reduced or destroyed by UV light and gamma irradiation, lipid solvents,b-propiolactone, formaldehyde, sodium hypochlo-rite, and phenolic disinfectants.

Geographical Distribution

EVD outbreaks occur primarily in remote villages in Central and West Africa, neartropical rainforests. The virus is transmitted to people from wild animals and spreads in the human population through human-to-human transmission. Since 2008, Restonebolavirus has been detected during several outbreaks of adeadly disease in pigs in the People's Republic of China and in Philippines, but noillness or death in humans from this species has been reported to date. On 8 August 2014 the World Health Organisation (WHO)declared the Ebola virus disease (EVD) outbreak in West Africa a Public Health Emergency of International Concern (PHEIC), stressing the need for international attention and collaboration to control the outbreak. At this moment (18 September 2014) a total of 5335 caseswith 2622 reported deaths have been notified, in Guinea, Liberia, and Sierra Leone. The imported EVD case inNigeria that resulted in a relatively small outbreak, and similar imported cases in the USA and Spain which at first appeared to have been well contained, but eventually lead to infection of healthcare workers, show the importance of adequate isolation methods, training of personnel and the adequate use of personal protective equipment (PPE). For the West Africa outbreak, the total number of cases is subject to change due to ongoing re classification, retrospective investigation and the availability of laboratory results. A second, non-related, EVD outbreak has been reported in the Democratic Republic of Congo with currently a total of 62 confirmed and suspected cases.

Reservoir

Despite extensive work, no filo virus vector has been identified. Ape-to-ape transmission may be responsible for the epizootic wave of this disease, although the fruit bat act as a reservoir for this disease. Fruit bats of the Pteropodidae

family are well thought-out to be the natural host of the Ebola virus. Although non-human primates have been a source of infection for humans, they are not thought to be the reservoir but rather an accidental host like human beings. Since 1994, Ebola outbreaks from the EBOV and TAFV species have been observed in chimpanzees and gorillas. RESTV has caused severe EVD outbreaks in macaque monkeys (Macaca fascicularis)farmed in Philippines and detected in monkeys imported into the USA in 1989, 1990and 1996, and in monkeys imported to Italy from Philippines in 1992.A recent study suggests that bats might be a reservoir for Ebola virus in Bangladesh. The study found antibodies against Zaire and Reston ebola viruses circulating in 3.5%of the 276 bats scientists screened in Bangladesh. Detection of antibodies to Ebola virus infection in Indonesian orangotans suggests the existence of multiple species of filo viruses or unknown filo virus-related viruses in Indonesia, some of which are serologically similar to African ebola viruses.

Pathogenesis and Transmission

After infection, development of disease is a complex interplay between virus, host and environment. Different case fatality rates (CFR) have been reported between the four human-pathogenic Ebola viruses. For EBOV the CFR ranges from 50-90% of the EVD cases. For the current outbreak, CFR is estimated to be around 50%, although there is some evidence of improved outcomes with intense symptomatic treatment. Ebola is spread through direct contact (through broken skin or unprotected mucous membranes in, for example, the eyes, nose, or mouth) with blood or body fluids (including but not limited to faeces, saliva, sweat, urine, vomit, breast milk, and semen) of a person who is sick with Ebola. Infection through intact skin is considered unlikely, although not excluded. The virus has been successfully isolated from skin (biopsy) and body fluids. Objects (like needles and syringes) that have been contaminated with the virus, infected fruit bats or primates (apes and monkeys), and possibly from contact with semen from a man who has recovered from Ebola (for example, by having oral, vaginal, or anal sex).The route of transmission seems to affect the disease out come. Ebola is not spread through the air or by water, or in general, by food. However, in Africa, Ebola may be spread as a result of handling bushmeat (wild animals hunted for food) and contact with infected bats. There is no evidence that mosquitos or other insects can transmit Ebola virus.

Only a few species of mammals (for example, humans, monkeys, and apes) have shown the ability to become infected with and spread Ebola virus. In Africa, infection has been documented through the handling of infected chimpanzees, gorillas, fruit bats, monkeys, forest antelope and porcupines found ill or dead or in the rainforest. Ebola then spreads in the community through human-to-human transmission, with infection resulting from direct contact (through broken skin or mucous membranes) with the blood, secretions, organs or other bodily fluids of infected people, and indirect contact with environments contaminated with such fluids. Burial ceremonies in which mourners have direct contact with the body of the deceased person can also play a role in the transmission of Ebola. Health-care workers have frequently been infected while treating patients with suspected or confirmed EVD. This has occurred through close contact with patients when infection control precautions are not strictly practiced. In the early EBOV outbreak in 1976, CFR after transmission by injection was 100% versus 80%in contact exposure cases. This has been confirmed ina non-human primate model, showing faster disease progression in animals infected via injection versus those that received an aerosol challenge.

Post-mortem studies of patients and experimentally infected animals showed infection of immune cells (macrophages, monocytes and dendritic cells), epithelial and endothelial cells, fibroblasts, hepatocytes and adrenal gland tissue. Hallmark characteristics of EVD, as in any VHF, are the bleeding manifestations although these are infrequently observed inthe current outbreak. Studies addressing the mechanism behind these coagulation abnormalities first showed that haemorrhage was most likely not a direct effect of endothelial cell infection, followed by cytolysis. Amore likely explanation seems to be an over expression of tissue factor in monocytes/macrophages resulting in(over)activation of the extrinsic pathway of coagulation followed by a consumptive coagulopathy and eventually disseminated intravascular coagulation.

Signs and Symptoms

EVD is a severe acute viral illness often characterized by the sudden onset of fever, intense weakness, muscle pain, headache and sore throat. Incubation period is usually 2 to 21 days. This is followed by vomiting, diarrhoea, impaired kidney and liver function, and in some cases, both internaland external bleeding. Around Day 5, most patients develop a maculopapular rash that is prominent on the trunk followed by desquamation in survivors. Central nervous system involvement is often manifested by somnolence, delirium, or coma. During the second week, the patient defervesces and improves markedly or dies in shock with multi organdys function, often accompanied by disseminated intra vascular coagulation, anuria, and liver failure. Convalescence may be protracted and accompaniedby arthralgia, orchitis, recurrent hepatitis, transversemyelitis, psychosocial disturbances, or uveitis. It also includes low white blood cell and platelet counts and elevated liver enzymes. People are infectious as long as their blood and secretions contain the virus. Men who have recovered from the disease can still transmit the virus through their semen for up to 7 weeks after recovery from illness.

Diagnosis

Diagnosing Ebola in a person infected for only a few days is difficult as the early symptoms, such as fever, are nonspecific to Ebola and are seen often in patients with more common diseases, such as malaria and typhoid fever. However, if a person has the early symptoms of Ebola, the patient should be secluded and public health professionals notified. Samples from the patient can then be collected and tested to confirm infection. It may take up to three days after symptoms start for the virus to reach detectable levels. The diagnosis of acute EVD is made by viral genome detection via RT-PCR. The virus is usually detectable 48hours after infection in both lethal and non-lethal cases. This suggests that a negative test result within the first 48hours after exposure does not rule out EBOV infection. Due to the quickness of the acute disease, serology does not play a role in diagnosis of acute EVD patients but maybe of use in epidemiological and surveillance studies. In common, IgM antibodies can be detected starting from two days after the first symptoms appear and disappear after30-168 days. IgG response is generally considered to start between day 6 and 18 post onset of illness and remains detectable for years. Antibody profile of the sera from patients with lethal disease as compared with those that survive is markedly distinct. This difference can serve as a predictive marker for the management of the patient since antibody responses strongly differ between lethal and survivor cases and it has been shown that deceased patients show a much lower or even absent antibody response compared with survivors.

Treatment

There is no FDA-approved treatment (e.g., antiviral drug) for Ebola. Symptoms and complications are treated as they appear. The following basic intrusions, when used early, can significantly improve the chances of survival:

- Providing intravenous fluids and balancing electrolytes (body salts)
- Maintaining oxygen status and blood pressure
- Treating other infections if they occur

Experimental treatments for Ebola are under expansion, but they have not yet been fully tested for safety or effectiveness. Retrieval from Ebola depends on good supportive care and the patient's immune response. People who recover from Ebola develop antibodies that last for at least 10 years, possibly longer. It isn't known if people who recover are immune for life or if they can become infected with a different species of Ebola. Some people who have recovered from Ebola have developed long-term complications, such as joint and vision problems. Ebola virus has been found in the semen of some men who have recovered from Ebola. It is possible that Ebola could be spread through sex or other contact with semen. It is not known if Ebola can be spread through sex or other contact with vaginal fluids from a woman who has had Ebola.

Prevention

While travelling to an area affected by an Ebola outbreak, make sureto:

- Practice careful hygiene. For example, wash your hands with soap and water or an alcohol-based hand sanitizer.

- Avoid contact with blood and body fluids.
- Do not handle items that may have come in contact with an infected person's blood or body fluids (such as clothes,bedding, needles, and medical equipment).
- Avoid funeral or burial rituals that require handling the body of someone who has died from Ebola.
- Avoid contact with bats and nonhuman primates or blood, fluids, and raw meat prepared from these animals.
- Monitor your health after you return for 21 days and seek medical care immediately if you develop symptoms of Ebola.

Healthcare workers who may be exposed to people with Ebola should follow these steps:

- Wear appropriate personal protective equipment (PPE).
- Practice proper infection control and sterilization measures.
- Isolate patients with Ebola from other patients.
- Avoid direct contact with the bodies of people who have died from Ebola.
- Notify health officials if you have had direct contact with the blood or body fluids of a person sick with Ebola.

CONCLUSION

Fast and extensive geographic spread of the current Ebola virusoutbreak are motives for increased alertness. Owing to the initial non-specific presentation ofEVD, the mixture of fever in combination with high-riskexposure isadequate to proceed with isolation and managementprotocols in patients who visited endemic areas. Presently, treatment approachescount on solely onthe early start of supportive care, where aggressive fluidreplacement therapy is proven to drastically improve thesurvival rates. Precise antiviral EVD treatment approachesare still in the experimental phase. All countries and clinicalcentres should be conscious of the potential for admission ofan EBOV infected person.

Author Contribution Statement

Pradip Kumar Prusty and Sasmita Panda conceived the idea. All authors contributed significantly in drafting the manuscript.

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Conflict of Interest

The authors declare that they have no conflict of interest.

REFERENCES

1. Isaacson, M; Sureau, P; Courteille, G; Pattyn, SR;. Clinical Aspects of Ebola Virus Disease at the Ngaliema Hospital, Kinshasa, Zaire, 1976.
2. WHO. Media Centre. Ebola virus disease. Fact sheet N°103. http://www.who.int/mediacentre/factsheets/fs103/en/.

3. WHO Global Alert and Response. Ebola Reston in pigs and humans in the Philippines – update, www.who.int/csr/don/2009_03_31/en/.
4. Olival KJ, Islam A, Yu M, Anthony SJ, Epstein JH, Khan SA, Khan SU, Crameri G, Wang LF, LipkinWI, Luby SP, Daszak P.; Ebola virus antibodies in fruit bats, Bangladesh. Emerg Infect Dis. 2013Feb;19(2):270-3. doi: 10.3201/eid1902.120524.
5. Nidom CA1, Nakayama E, Nidom RV, Alamudi MY, Daulay S, Dharmayanti IN, Dachlan YP, Amin M,Igarashi M, Miyamoto H, Yoshida R, Takada A. Serological evidence of Ebola virus infection in Indonesianorangutans. PLoS One. 2012;7(7): e40740. doi: 10.1371/journal.pone.0040740. Epub 2012 Jul 18.
6. M. Goeijenbier, J.J.A. van Kampen, C.B.E.M. Reusken, M.P.G. Koopmans, E.C.M. van Gorp. Ebola virus disease: a review on epidemiology,symptoms, treatment and pathogenesis. The Journal of Medicine. November2 014;72(9):442-448

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RESEARCH ARTICLE

Cancer: Fight the Fight, Find the Cure

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ABSTRACT

Cell is the structural and functional unit of living organism. Cell is the basic unit of life which exhibits an advanced cellular organization in case of eukaryotes by containing diverse cell organelles. A multicellular organism grows well when all its molecular events regulating the cell growth and division are tightly regulated and thus the cellular environment thrives in a normal fashion. In rare cases, a normal cell suddenly behaves abnormally as if it became a rebel and shows reluctance towards the fundamental rules that govern cell growth and reproduction. Then they start dividing hastily, invading other tissues, grabbing resources, and even insome cases leading into killing the body in which it lives. To dissect the causes that leads the cell to unfollow the basic principles can be understood only, when we can unsolved the mysteries related to the normal functions of cell growth and reproduction. Cutting edge research in basic and applied biosciences field has provided detailed and specific information about the molecules and processes that plays a pivotal role in the cell cycle involving cell division, cell growth, cell differentiation that specifies the cells with their distinct roles. This detailed understanding provides an insight into various mechanisms that triggers cancer.The tight regulation of cell cycle plays a very important role in not allowing the normal cells to become cancerous thus loss of control of the cell cycle is one of the crucial steps in development of cancer.Even though, until now a number of different type of cancer diseases have been discovered, but they all share an important characteristic in common: they are abnormal cells where the normal cell division process is disturbed. Cancer is a consequence of switching of normal cells to abnormal cells which are triggered by various factors like inherited mutations, environmental factors such asUV light, X-rays, chemicals, tobacco products, and viruses. Studies suggests that most cancers are an outcome of various synchronized events and thus evolving the cell

through a series of premalignant stages into an invasive cancer.The visible symptoms of cancer may appear years after initial event and the development of cancer. A high throughput sophisticated and reliable molecular biological techniques may help in the diagnosis of potential cancers in the early stages, well before the formation of any visible phenotypic symptoms.

Keywords: Cell, cancer, invasive, symptoms.

INTRODUCTION

Cancer is an outcome of a series of molecular events which are aimed to alter the physiology of normal cells by disabling the basic processes that prevent cell overgrowth and the invasion of other tissues. Then these cells are able to divide and grow even in the presence of signals which usually are responsible for inhibiting cell growth and division. As a result, these abnormally growing cells develop new features including changes in their cell structure, production of new bimolecular including enzymes, decreased cell adhesion thus making them gradually free to move. These heritable changes thus allow the progeny to divide and grow as their parent cell which are unaffected by the presence of normal cells that typically inhibit the growth of nearby cells. These changes allow the cancer cells to spread and invade other tissues. As mentioned, the irregularities foundin cancer cells usually result from mutations in protein-encoding genes that regulate the cell division. Over a period of time more genesare self-mutated. This is so because the DNA repairing genes that encode the DNA repairing proteins are themselves not functioning normally because they are also mutated. As a result of which, mutations begin to accumulate in the cell, promoting aberrationsin that cell and the progenies. Some of these mutated cells die, but other alterations may provide the abnormal cell a selective benefit that permits it to multiply much more rapidly than the normal cells. As long as these cells are restricted to their original location, they are considered as benign in nature; if they become invasive, then they are considered as malignant. Cancer cells in case of malignant tumors can often metastasize, sending cancer cells to distant sites in the body where new tumors may result.

Genetic basis of Cancer

A small fraction of the approximately 35,000 genes in the human genome have been associated with cancer. Variations in the same gene are associated with different forms of cancer thus resulting into a number of cancer types relative to the number of cancer related genes. These malfunctioning genes can be chiefly classified into three groups. The first group, called proto-oncogenes, produces protein products that usuallyboost cell division or inhibit normalcell death. The mutated forms of these genes are called oncogenes.The second group, called tumor suppressors, makes proteins thatnormally prevent cell division or cause cell death. The third group contains DNA repair genes, which help prevent mutations that leadto cancer.Proto-oncogenes and tumor suppressor genes work much like an antagonist, opposing each other. Controlled cell growth is maintained by tight regulation ofproto-oncogenes, which accelerate growth, and tumor suppressor genes,which slow cell growth. Mutations that produce oncogenes accelerategrowth while those that affect tumor suppressors prevent the normalinhibition of growth. Either case, leads to uncontrolled cell growth.

Oncogenes and Signal Transduction

In normal physiological cells, proto-oncogenes encode the proteins that send asignal to the nucleus to arouse cell division. These signaling proteins act in a series of downstream steps called as signal transduction cascade or pathway. This cascade includes a membrane receptor for the signal molecule which acts as a stimulus, intermediary proteins that carry the signal through the cytoplasm, and finally the transcription factorsin the nucleus that activate the genes for cell division. In each step of the pathway, one factor or protein activates the downstream molecule ad itself gets recycled for being used in next round. Oncogenes are altered versions of the proto-oncogenes that code for these signaling molecules. The oncogenes activate the signaling cascade endlessly,ensuingan increased production of

factors that stimulate growth. For example, MYC is a proto-oncogene that codes for a transcription factor. Mutations in MYC convert it into an oncogene which is roughly associated with a large variety of cancers. RAS is another oncogene that usually functions as an "on-off" switch in the signal cascade. Mutations in rascausethe signaling pathway to remain in "on," condition thus leading to uncontrolledcell growth. About thirty percent of tumors including lung, colon,thyroid, and pancreatic carcinomas have a mutation in RAS.The renovation of a proto-oncogene to an oncogene may occur by various molecular mechanisms including mutation of the proto-oncogene, by rearrangement of genes in thechromosome that moves the proto-oncogene to a new location, or byan increase in the number of copies of the normal proto-oncogene. Occasionally a virus may insert its DNA in or near the proto-oncogene, instigating it to become an oncogene. The result of any of these events isan altered form of the gene, which contributes to cancer. Most oncogenes are dominant mutations; a single copy of this gene is enough for expression of the growth trait. This is also a "gain offunction" mutation since the cells with the mutant form of theprotein have gained a new function absent in cells with thenormal gene. Likewise, one copy of an oncogene is sufficient to cause variations in cell growth. The occurrence of anoncogene in a germ line cell (egg or sperm) marks in an inherited predisposition for tumors in the offspring. Though, a single oncogeneis not usually sufficient to cause cancer, so inheritance of an oncogenedoes not necessarily result in cancer.

Tumor Suppressor Genes

The proteins produced from the tumor suppressor genes usually inhibit cell growth, preventing tumor formation. Mutations in these genes result in cells which are devoid of normal inhibition of cell growth anddivision. The products of tumor suppressor genes may act at the cellmembrane, in the cytoplasm, or in the nucleus. Mutations in thesegenes result in a loss of function (that is, the ability to inhibit cellgrowth) thus they are usually recessive.Unlike oncogenes, in case of the tumor suppressor genes, the trait is notexpressed unless both copies of the normal gene are mutated.The how is it that both genes can become mutated. In few cases, the first mutation is already present in a germ line cell (egg or sperm); thus, allthe cells in the individual inherit it. Since the mutation is recessive,the trait is not expressed. In future a mutation may occur in the second copy ofthe gene in a somatic cell. In that cell both copies of the gene are mutated and thus the cell develops uncontrolled growth. An example ofthis is hereditary retinoblastoma, a serious cancer form of the retina that happens in early childhood.

When one parent carries a mutation in onecopy of the RB tumor suppressor gene, it is transmitted to offspringwith a fifty percent probability. About ninety percent of the offspringwho receive the one mutated RB gene from a parent also develop amutation in the second copy of RB, usually very early in life. Theseindividuals then develop retinoblastoma. Not all cases of retinoblastoma are hereditary: chances are there that they can occur by mutation of bothcopies of RB in the somatic cell of the individual. As retinoblastsare rapidly dividing cells and there are thousands of them, there is ahigh incidence of a mutation in the second copy of RB in individualswho inherited one mutated copy. This disease worries only youngchildren because only individuals younger than about eight years old have retinoblasts. In adults, however, mutations in RB may lead to a susceptibility to several other forms of cancer.

Some other cancers associated with defects in tumor suppressor genesinclude familial adenomatous polyposis of the colon (FPC), whichresults from mutations to both copies of the APC gene; hereditarybreast cancer, resulting from mutations to both copies of BRCA2; andhereditary breast and ovarian cancer, resulting from mutations to bothcopies of BRCA1. These cancer typesadvise that heredity is a significant factor in cancer but a number of cancers are irregular with noindication of a hereditary component. Cancers involving tumorsuppressor genes are often hereditary because a parent may provide agerm line mutation in one copy of the gene. This may lead to a higherfrequency of loss of both genes in the individual who inherits themutated copy than in the general population. However, mutations inboth copies of a tumor suppressor gene can occur in a somatic cell, sothese cancers are not always hereditary. Somatic mutations that lead toloss of function of one or both copies of a tumor suppressor gene maybe because of several environmental factors.

DNA Repair Genes

This group of genes are associated with the DNA repair processes and maintenance of chromosome structure. Abiotic environmental factors like ionizing radiation, UV light, and chemicals, can lead to the damage of DNA. Errors although a very rare event which occur during DNA replication can also lead to mutations.Gene products of DNA repair genes are involved in repairing any damage to chromosomes, thereby curtailing the frequency of mutations in the cell. But, when a DNA repair gene is mutated its product isno longer available thus, preventing DNA repair and lettingfurther mutations to occur in the cell. These mutations can surge the frequency of a healthy cell to become cancerous. For example, a defect in a DNA repair gene called XP (Xerodermapigment sum) results in individuals who are very sensitive to UV light and have a high risk of suffering with a various types of skin cancer. There are seven XP genes, whose productseliminate DNA damage caused by UV light and other carcinogenic agents. Another example of a disease that is allied with lossof DNA repair is Bloom syndrome, an inherited disorder that leads to increased risk of cancer, lung disease, and diabetes. The DNA repair geneBLM, is required for maintaining the stable structure of chromosomes. Individuals with Bloom syndrome have ahigh frequency of chromosome breaks and interchanges, which can lead to the activation of oncogenes.

Cell Cycle

Normal healthy cells grow and divide in a tidy, well regulated fashion, in accordance with the cell cycle comprised of several check-points. Mutations in proto-oncogenes or in tumor suppressor genes allow a cell to grow and divide without the usual controls imposed by the cell cycle and thus making the healthy cell viable to cancerous features. A number of proteins are involved in controlling the timing of the events in the cell cycle, which is tightly regulated to make sure that cells divide only when needed. Any kind of damage inthis regulation is the hallmark of cancer. The cyclin-dependent kinases are major control switches of the cell cycle. Each cyclin-dependent kinase forms a complex with a specificcyclin, a proteinthat binds and activates the cyclin-dependent kinase. The kinase portion of the complex is an enzyme that supplements a phosphate to various downstream proteinsrequired for progression of a cell through the cycle. These addedphosphates alter the structure of the protein and can activate orinactivate the protein, depending on its function.

There are specificcyclin-dependent kinase/cyclin complexes at the entry points into theg1, S, and M phases of the cell cycle, as well as other factors thathelp prepare the cell to enter S phase and M phase. One of the important protein in the cell cycle is p53, a transcription factorthat binds to the DNA, activating transcription of a protein called p21. P21 then blocks the activity of a cyclin-dependent kinase required for progression through G1. This blocking allows the cell to repair the DNA before it is replicated. If incase, thednadamage is so extensive that it cannot be repaired, p53 triggersthe cell to commit suicide. The most common mutation leading tocancer is in the gene that makes p53. Li-Fraumeni syndrome, an inherited predisposition to multiple cancers, outcomes from a germ line(egg or sperm) mutation in p53. Other protein factors that halts the cell cycleby inhibiting cyclin dependent kinases are p16 and RB. All of theseproteins, including p53, are tumor suppressors.Cancer cells do not stop dividing whereas normal healthy cells are not allowed to divide continuously in an unregulated fashion. With reference to cell division, normal cells vary from cancer cellsin at least four ways.

• Normal cells require external growth factors to divide. When production of these growth factors is inhibited by normal cell regulation, the cells stop dividing. But, cancer cells have lost the needfor positive growth factors, so they divide irrespective of the presence of these factors. Consequently, they do not behave as part ofthe tissue as they have become independent cells.

• Normal cells show contact inhibition. They respond tocontact with other cells by ceasing cell division. Therefore, cells candivide to fill in a gap, but they stop dividing as soon as there areenough cells to fill the gap. This characteristic is absent in cancer cells which continue to grow after they touch other cells, leading to the formation ofalarge mass of cells.

• Normal cells age and die, and are replaced in a controlled andorderly fashion by new cells. Apoptosis is the normal,programmed cell death. Each time the chromosome replicates, the telomeres shorten. In growing cells,

theenzyme telomerase replaces these lost ends. Adult cells lack telomerase, limiting the number of times the cell can divide.Whereas, telomerase is activated in cancer cells, allowing anunlimited number of cell divisions.

•Normal cells stop to divide and die when there is DNA damage orwhen cell division is abnormal. Cancer cells continue to divide,even when there is a huge amount of DNA damage and when thecells are abnormal. These progeny cancer cells contain theabnormal DNA, thus as the cancer cells continue to divide theyaccumulate more and more damaged DNA.

Cause of Cancer

Cancer can be multifactorial, meaning there is no single cause in for any one type of cancer.

Cancer-causing substances (carcinogens): - Mutation or changes to the gene, such as damage or loss, can alter how that cell behaves. For example, a mutation may result in the production of too much proteins or that protein may not be made at all. Something that damages a cell, changing its behavior and makes it more likely to be cancerous is called a 'carcinogen'.

Age: - Many types of cancer become more prevalent with age. The longer the people live, the more exposure there is to carcinogens and the more time there is for genetic changes or mutations to occur within their cells thus increasing the risk of cancer.

Genetics: - Prevailing model for cancer development reveals that mutations in genes for tumor suppressors and oncogenes lead to cancer. However, it may not be that too simple, as the prevailing model fails to explain the genetic diversity among cells within a single tumor and does not adequately explain many chromosomal aberrations typical of cancer cells. An alternate model proposes that there are “master genes” controlling cell division. A mutation in a master gene leads to abnormal replication of chromosomes, triggering whole sections of chromosomes to be missing or duplicated. This leads to a change in gene dosage, so cells produce too little or too much of a specific protein. If the chromosomal aberrations affect the amount of one or more proteins controlling the cell cycle, such as growth factors or tumor suppressors, the result may be cancer. There is also strong evidence that the excessive addition of methyl groups to genes involved in the cell cycle, DNA repair, and apoptosis is characteristic of some cancers.

The immune system: - People who have weakened immune systems are more disposed to developing some types of cancer. This includes people who have had organ transplantsand take drugs to suppress their immune systems to stop organ rejection, peoplewho have HIV or AIDS, or other medical conditions which reduce their immunity. Certain lifestyles and environmental factors also can cause mutations that can lead to cancer. Lifestyle and environmental causes are to a large extent controllable or avoidable. Examples include:

- Bodyweight, diet and physical activity - Experts estimate that maintaining healthy bodyweight, making changes to our diet and doing regular physical activity could preventcancer. Many people consume too much red and processed meat and not enough fresh fruit and vegetables. This type of diet is known to increase the risk of cancer
- Overweight or obesity - Overweight or obese people have ahigher risk of bowel and pancreatic cancer, probably due to a tendency towards higher insulin levels. Obesity can also increase therisk of cancer of the oesophagus (oesophageal cancer), kidney and gallbladder cancer, aswell as breast or womb (uterine) cancer in women.
- Alcohol - The evidence that all types of alcoholic drinks are a cause of a number of cancers is now stronger. Alcohol can increase the risk of a number of cancers, including mouth, throat (like pharyngeal cancer), laryngeal and cancer of the food pipe, liver cancer.
- Tobacco – Tobacco smoke contains at least 80 different carcinogenic agents. When smoke is inhaled the chemicals enter the lungs, pass into the blood stream and are transported throughout the body. Thus smoking or chewing tobacco not only causes lung cancer and mouth cancers, but is also related to many other cancers.

- Ionising radiation – Manmade sources of radiation can cause cancer and are a risk for people associated with it. The main risk is however, extended and unprotected exposure to ultraviolet radiations from the sun which can lead to melanoma and skin malignancies. Fair skinned people, those with lot of moles or who have a relative who has had melanoma or non-melanoma skin cancer, are at utmost risk. Curie, who discovered radium, paving the way for radiation therapy for cancer, died of cancer herself as a result of radiation exposure in her research.
- Work place hazards - Some people risk being exposed to a cancer causing substance because of the work they are associated with. Workers in the chemical dye industry havebeen found to have a higher incidence than normal for bladder cancer. Asbestos is a well-known work place cause of cancer, particularly a cancer called mesothelioma, which most commonly affects the covering of the lungs (pleura).
- Infection – Some cancers can also be caused by infection with a virus. The virus cancause changes in cells that make them more likely to become cancerous. Examples include cervical cancer, linked to the Human Papilloma Virus, primary liver cancer which can be caused by the Hepatitis B and C virus andlymphomas linked to the Epstein-Barr virus. Previously, bacterial infections have not been thought of as cancer causing agents. But studies have shown that people who have helicobacter pylori infection of their stomach, develop inflammation of the stomach lining, which increases the risk of stomach cancer.

There may be multiple mechanisms leading to the development of cancer. This, further complicates the difficult task of determining what causes cancer.

Tumor Biology

Cancer cells act as independent cells, growing in uncontrollable fashiontoform tumors. Tumors grow in a series of steps. The first step ishyperplasia, meaning that there are too many cells resulting fromuncontrolled cell division. These cells look normal, but changeshave occurred that result in some loss of control of growth. Thesecond step is dysplasia, resulting from further growth, accompaniedby abnormal changes to the cells. The third step requires additionalchanges, which result in cells that are even more abnormal and cannow spread over a wider area of tissue. These cells begin to lose theiroriginal function; such cells are called anaplastic. At this stage, since the tumor is still restricted within its original location (calledin situ) and is not invasive, it is not considered malignant but it ispotentially malignant. The last step occurs when the cells in the tumormetastasize, which means that they can invade surrounding tissue,including the bloodstream, and spread to other locations. This is themost serious type of tumor, but not all tumors progress to this point.Non-invasive tumors are said to be benign.The type of tumor that forms depends on the type of cell that wasinitial site of infection. There are five types of tumors.

•**Carcinomas** result from altered epithelial cells. This arises from the epithelial cells (the lining of cells that helps protect or enclose organs). Carcinomas may invade the surrounding tissues and organs and metastasize to the lymph nodes and other areas of the body. The most common forms of cancer in this group are breast, prostate, lung and colon cancer.

•**Sarcomas** result from changes in muscle, bone, fat, or connective tissue. A type of malignant tumor of the bone or soft tissue (fat, muscle, blood vessels, nerves and other connective tissues that support and surround organs). The most common forms of sarcoma are leiomyosarcoma, liposarcoma and osteosarcoma.

•**Leukemia** results from malignant white blood cells.Leukaemia is a cancer of the white blood cells and bone marrow, the tissue that forms blood cells. There are several subtypes; common are lymphocytic leukaemia and chronic lymphocytic leukaemia.

•**Lymphoma** is a cancer of the lymphatic system cells that derive from bone marrow. Lymphoma is a cancer of the lymphatic system, which runs all through the body, and can therefore occur anywhere. The two main forms are non-Hodgkin's which begins with uncontrolled growth of the - white blood cells -lymphocytes - of the immune system) and Hodgkin's lymphoma in which cells of the lymph nodes become cancerous.

•**Myelomas** are cancers of specialized white blood cells that make antibodies.

Angiogenesis

Any cell whether it is healthy or cancerous requires nutrients andoxygen in order to grow. All living tissues are adequately supplied withcapillary vessels, which circulates nutrients and oxygen to every cell. Astumorsexpand; the cells in the center no longer receive nutrients from the normal blood vessels. To provide a blood supply for all the cells inthe tumor, it must form new blood vessels to supply the cells with nutrients and oxygen. Angiogenesis, is a process where tumor cells make growth factors which induce formation of newcapillary blood vessels. The cells of the blood vessels that divide to make new capillary vessels are inactive in normal tissue; however, tumorscan make angiogenic factors, which activate these blood vessel cellsto divide. Without the additional blood supplied by angiogenesis, tumors cannot grow larger and also cannot spread, or metastasize to new tissues. Tumor cells can cross through the walls of the capillaryblood vessel at a rate of about one million cells per day. Still not all cells in a tumor are angiogenic. Both angiogenic and non-angiogenic cells in a tumor cross into blood vessels and spread.

However, non-angiogenic cells give rise to dormant tumors when theygrow in other locations. In contrast, the antigenic cells quickly establish themselves in new locations by growing and producing new blood vessels, resulting in rapid growth of the tumor. Tumors produce angiogenic factors. An oncogenecalled BCL2 has been shown to greatly surge the production of apotent stimulator of angiogenesis. There are severalangiogenic factors and production of many of these is increased by a variety of oncogenes.Thus, oncogenes in some tumor cells allow those cells to produceangiogenic factors. The progeny of these tumor cells will also produceangiogenic factors, so the population of angiogenic cells willincreases the size of the tumor increases. Angiogenesis is critical for the progression of dormant tumors into cancer.

Signs and Symptoms

As there are so many different types of cancer, the symptoms are varied and depend on where the disease is located. However, there are some key signs and symptoms, including:

•Lumps: - some cancers can be felt through the skin. Cancerous lumps are often painless and may increase in size as the cancer progresses.

•Coughing, breathlessness: - persistent coughing episodes and breathlessness can beassociated with lung cancer.

•Changes in bowel habit: - symptoms of bowel cancer may include blood in the stoolsand a change in bowel habits such as constipation and diarrhea.

•Bleeding: - any unexpected bleeding can be a sign of cancer:

O Bleeding from the anal passage may be a sign of bowel cancer.

O Bleeding from the cervix may be a sign of cervical cancer.

O Blood present in the urine may be a sign of kidney or bladder cancer.

•Unexplained weight loss: - a large amount of unexplained weight loss over a short period of time (a couple of months) can be a sign of cancer.

•Fatigue: - fatigue is extreme tiredness and a severe lack of energy. If fatigue is due to cancer, sufferers normally also have other symptoms.

Detecting and Diagnosing Cancer

Imaging techniques such as MRI, X-rays, CT, and ultrasound are the most common techniques which can provide an image of a tumor. Endoscopy allows to look for tumors in organs such as the stomach, colon, and lungs. Most of these techniques are used to detect visible tumors, which must then be removed by biopsy and examined microscopically by a pathologist. Then the aberrations in the cells in terms of their shape, size, and structure, especially the nucleus need to be sorted out. Basedon investigation of the tumor cells, the tumorcan be classified as benign or malignant, and also the stage of development of tumor can be defined whether in early or late stage. Tumor markers proteins are found more frequently in the blood ofindividuals with the tumor than in normal individuals. These are notideal compounds for diagnosing of cancer for two reasons. First, individuals without cancer may have elevated levels of the marker,leading to false positives. Second, tumor markers are not

sufficientlyelevated in all individuals with cancer to allow their detection. Thisleads to false negatives. One of the most commonly used tumormarkers is prostate-specific antigen (PSA). It is present in all adultmales, but its level is amplified after both benign and malignantchanges in the prostate. Thus, high levels of PSA indicate onlythat further tests are prerequisite to determine whether the condition iscancer. If prostate cancer is diagnosed, the levels of PSA can help todetermine the effectiveness of treatment and detect recurrence.CA125 is another tumor marker, which is produced by a number ofdifferent cells, particularly ovarian cancer cells. It is used primarily tomonitor the treatment efficacy of ovarian cancer. When the cancer isresponding to treatment, CA125 levels drop. It is not used as a routinetest for ovarian cancer as many common conditions that causeinflammation also increase the level of CA125, leading to a highfrequency of false positives.

The earlier a cancer is found the more effectively it can be treated;however, early stage cancers typically produce no symptoms. Scientistsare evolvingmolecular techniques to detect very early cancer. Usingtechniques such as mass spectrometry, they are also developing specificblood tests to identify a pattern of new proteins in the blood of individuals with a particular type of cancer. Scientists are also developing DNA microarrays to identify genesexpressed in particular types of cancer cells. With the sequencing of the human genome and the mapping ofsingle nucleotide polymorphisms (snps), it may be possible to diagnose particular cancers by identifying cellswith known gene alterations. In 2002 scientists detected ovarian cancerby testing blood for the presence of DNA released by tumor cells. Theylooked for changes in certain alleles at eight snpsthat arecharacteristic of cancer. By using this technique, they could successfullyidentified eighty-seven percent of patients known to have early-stageof ovarian cancer and ninety-five percent of those with late-stageovarian cancer. The capability to determine which genetic alterations arerelated with various cancers unlocks the possibility of recognizingcancerous cells while the cancer is in an early, treatable stage.

Treatments

Treatment of cancer depends on the type of cancer, its location, and its state of development. **Surgery** is used to remove solid tumors. This treatment may be necessary for early stage cancers and benign tumors. **Radiation** treatment destroys cancer cells with high-energy rays targeted directly to the tumor site. It acts mainly by damaging DNA and preventing its replication. Therefore, it preferentially kills cancer cells. It also kills some normal cells, predominantly those that are dividing. Surgery and radiation treatment are often used together. **Chemotherapy** drugs are toxic compounds that target quickly growing cells. Many of these drugs are specially designed to restrict the synthesis of precursor molecules needed for DNA replication; they interfere with the ability of the cell to complete the S phase of the cell cycle. Other drugs cause extensive DNA damage, which stops replication. A class of drugs known as spindle inhibitors stops cell replication early in mitosis. During the mitosis, chromosome separation requires spindle fibers composed of microtubules. Spindle inhibitors stop the synthesis of microtubules. Since, most adult cells don't divide often; they are less sensitive to these drugs than are cancer cells.

Chemotherapy drugs also destroy certain adult cells that divide more rapidly, like those that line the gastrointestinal tract, bone marrow cells, and hair follicles. This results in some of the side effects of chemotherapy, including gastrointestinal distress, low white blood cell count, and hair loss.Although cancer cells have lost some of the normal responses togrowth factors, some cancer cells still require hormones for growth.Hormone therapy for cancer tries to starve the cancer cells ofthese hormones. This is typically done by drugs that block the activityof the hormone, although some drugs can block synthesis of thehormone. For example, some breast cancer cells require estrogen forgrowth. Drugs that block the binding site for estrogen can slow thegrowth of these cancers. These drugs are called selective estrogenreceptor modulators (serms) or anti-estrogens. Tamoxifen andRaloxifene are examples of this type of drug. Likewise, testosterone (anandrogen hormone) stimulates some prostate cancer cells. Selectiveandrogen receptor modulators (sarms) are drugs that block thebinding of testosterone to these cancer cells, inhibiting their growthand possibly preventing prostate cancer. Newer chemotherapeutic drugs target specific, active proteins or processes in cancer cell signal transduction pathways, such as receptors, growth factors, or kinases. As the targets are cancer-specific proteins, the faith is that these drugs will be much less toxic to normal cells than conventional cancer

drugs. Chemotherapy may fail because the cancer cells become resistant to the therapeutic drugs. One of the characteristics of cancer cells is a high frequency of mutation. In the presence of toxic drugs, cancer cells that mutate and become resistant to the drug will survive and multiply in the presence of the drug, producing a tumor that is also resistant to the drug. So many a times, combinations of chemotherapy drugs are given at the same time. This decreases the probability that a cell will develop resistance to several drugs at once. However, such multiple resistances do occur. Some drug-resistant cancer cells express a gene called MDR1 (multiple drug resistance). This gene encodes a membrane protein that can not only prevent some drugs from entering the cell, but can also expel drugs already in the cell. Another hopeful target for cancer therapy is angiogenesis.

Numerous drugs, including some naturally occurring compounds, have the ability to inhibit angiogenesis. Two compounds in this class are angiostatin and endostatin, both are derived from naturally occurring proteins. These drugs prevent angiogenesis by tumor cells, restricting tumor growth and preventing metastasis. Advantage of angiogenesis inhibitors is that, because they do not target the cancer cells directly, there is less chance that the cancer cells will develop resistance to the drug. Immunotherapy includes several techniques that use the immune system to attack cancer cells or treat the side effects of some types of cancer treatment. A technique called chemoimmunotherapy attaches chemotherapy drugs to antibodies that are specific for cancer cells. The antibody then carries the drug directly to cancer cells without harming normal cells, reducing the toxic side effects of chemotherapy. A similar strategy, radioimmunotherapy, couples specific antibodies to radioactive atoms, thereby targeting the deadly radiation specifically to cancer cells.

Cancer seems to result from a mixture of genetic changes andenvironmental factors. Lifestyle that minimizes exposure toenvironmental carcinogens is one effective means of preventingcancer. Individuals who restrict their exposure to tobacco products,sunlight, and pollution can greatly decrease their risk of developingcancer. Many foods contain antioxidants and other nutrients that mayhelp to prevent cancer. The National Cancer Institute recommends adiet with large amounts of colorful fruits and vegetables. These foodssupply sufficient amounts of vitamin A, C, and E, as well asphytochemicals and other antioxidants that help to prevent cancer.Vaccines are alsopotential candidates for prevention of cancer. It appears that vaccines such as hepatitis B vaccine, papillomavirus vaccine may play a crucial role in minimizing the risk of liver cancer and cervical cancer (precancerous lesions) respectively.

CONCLUSION

By here and now, we discern that cancer is not simply the localized lumps andbumps that we have been programmed to accept through the years.Cancer in the adult can often be seen as a deteriorating processwith symptoms representative of underlying systemic dysfunction.There are countlessfactors, including emotional, diet, drugs and chemicals, infections,genetic mutation and environmental pollutants.Conventional treatments look at cancer as a disease state. Thenatural-oriented doctor views cancer as a set of symptoms reflectingunderlying disease.The conventional treatment of surgery, radiation and chemotherapyhas been the cornerstone of cancer treatment over the past severaldecades. Less toxic and target-specific chemotherapeutic agents are being developed. Furtherresearch and clinical studies are also being conducted on naturaltherapies.The success of a treatment often depends on the stageof cancer, the age, the immunity status, and the tumor responserate of the patient.As more research is carried out new therapies will be found.Regrettably, most cancer patients do not have time to wait.Sometimes, they are only given a few more months to live and left behind with an unsolved question why did this happen to me?

Author Contribution Statement

Gagan Kumar Panigrahi and Annapurna Sahooconceived the idea. All authors contributed significantly in drafting the manuscript.

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Conflict of Interest

The authors declare that they have no conflict of interest.

REFERENCES

1. Schneider, K. 2001. Counseling about cancer: Strategies for genetic counseling. 2d ed. New York: John Wiley & Sons.
2. Bahls, C., and M. Fogarty. 2002. Reining in a killer disease. The Scientist 16[11]:16. An outline of several approaches to controlling cancer.
3. Gibbs, W. Wayt. 2003. Untangling the roots of cancer. Scientific American, July, 57–65. New evidence challenges old theories of how cancer develops.
4. Kling, Jim. 2003. Put the blame on methylation. The Scientist16[12]:27–28. Gene silencing by methylation rather than by gene mutation may create some cancer cells.
5. mccook, A. 2002. Lifting the screen. Scientific American, June, 16–17. Developing protein "fingerprints" to screen for cancer.
6. Rayl, A. J. S., and Lewis, R. 2001. In cancer research, diet and exercise roles strengthen. The Scientist 15[20]:17. Evidence for the importance of lifestyle in preventing cancer.
7. Veggeberg, S. 2002. Fighting cancer with angiogenesis inhibitors. The Scientist 16[11]:41. Discussion of a class of drugs that helps to prevent angiogenesis.
8. Wilson, J. F. 2001. A dual role for CDK inhibitors. The Scientist 16[6]:20. Discusses approaches to cancer treatment using cells' cycle inhibitors.
9. Wilson, J. F. 2002. Elucidating the DNA damage pathway. The Scientist 16[2]:30. How researchers have deciphered the role of DNA damage repair in cancer.

Table 1. Some Genes Associated with Cancer

NAME	FUNCTION	EXAMPLES of Cancer/Diseases	TYPE of Cancer Gene
APC	Regulates transcription of target genes	Familial Adenomatous Polyposis	Tumor suppressor
BCL2	Involved in apoptosis; stimulates angiogenesis	Leukemia; Lymphoma	Oncogene
BLM	DNA repair	Bloom Syndrome	DNA repair
BRCA1	May be involved in cell cycle control	Breast, Ovarian, Prostatic, & Colonic Neoplasms	Tumor suppressor
BRCA2	DNA repair	Breast & Pancreatic Neoplasms; Leukemia	Tumor suppressor
HER2	Tyrosine kinase; growth factor receptor	Breast, Ovarian Neoplasms	Oncogene

MYC	Involved in protein-protein interactions with various cellular factors	Burkitt's Lymphoma	Oncogene
P16	Cyclin-dependent kinase inhibitor	Leukemia; Melanoma; Multiple Myeloma;	Tumor suppressor
P21	Cyclin-dependent kinase inhibitor	Pancreatic Neoplasms	Tumor suppressor
P53	Apoptosis; transcription factor	Colorectal Neoplasms; Li-Fraumeni Syndrome	Tumor suppressor
RAS	GTP-binding protein; important in signal transduction cascade	Pancreatic, Colorectal, Bladder Breast, Kidney & Lung Neoplasms; Leukemia; Melanoma	Oncogene
RB	Regulation of cell cycle	Retinoblastoma	Tumor suppressor
SIS	Growth factor	Dermatofibrosarcoma; Meningioma	Oncogene
XP	DNA repair	Xerodermapigmentosum	DNA repair

Table 2. Some Drugs Used in the Treatment of Cancer

CLASS	MECHANISM
Selective estrogen receptor modulators	Blocks the binding site for estrogen;
(SERM); (Tamoxifen and Raloxifene)	Can slow the growth of estrogen-stimulated cancers
Selective androgen receptor modulators	Blocks the binding site for testosterone;
(SARM)	Can slow the growth of testosterone-stimulated cancers
Spindle inhibitors	Stops cell replication early in mitosis
Farnesyltransferase inhibitors	Blocks the addition of a farnesyl group to RAS,
	Preventing its activation
Gleevec®	Binds to abnormal proteins in cancer cells, blocking their action
Angiogenesis inhibitors	
(endostatin, angiostatin)	Prevent angiogenesis by tumor cells
Immunostimulants	Enhance the normal immune response
(interleukin 2, alpha interferon)	Antibody that binds to HER2 receptor on tumor cells,
Herceptin®	Preventing the binding of growth factors

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RESEARCH ARTICLE

Aquaponics: An Innovative Approach of Integrated Farming in Modern Era

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ABSTRACT

Aquaponics is a typical bio-integrated system that forms a critical link between the recirculating aquaculture with hydroponic vegetable, flower, and/or herb production. It establishes a type of symbiotic relationship between aquatic animals with that of plants with in a system. Recent advances by researchers all around the globe have curved aquaponics into a working model of sustainable food production. This innovation named aquaponics respects principle of sustainability as well as gives a possibility to increase economical efficiency with an additional productivity. For the improvement of man's health we must reconsider the agricultural sciences in such a way that we can develop technologies friendly for the environment.

Keywords: Aquaponics, aquaculture, hydroponic, productivity.

INTRODUCTION

Aquaponics is the merger of aquaculture or fish cultivation and hydroponics or plant farming devoid of soil. The escalating rate of scientific and technological innovation has kept researchers in an unremitting struggle to update themselves with the latest codes of practices, technologies and scientific breakthroughs. The need and exigency of sustainable development for the aquaculture is beyond the thought. Increased productivity with reduced ecological impact, integration between production systems and reduced use of chemicals are some of the leading principles that more sustainable fish production needs to follow (Diver S, 2006). The safety of food for human consumption is

alarming on a worldwide level. Aquaculture represents fish farming, one system where commercial fishes are reared in containers, ponds or tanks. Hydroponics generally refers to the production of plants without soil. Plant roots are able to grow in a nutrient solution with or without an artificial medium for mechanical support (Pantanella E, 2008). Hydroponics is one of the plant culture techniques, which enables plant growth in a nutrient media with the mechanical support of inert substrata. Hydroponics is considered as a promising technique not only for plant physiology experiments but also for commercial production (Hutchinson W, 2004). Both aquaculture and hydroponics have some negative aspects. Hydroponics requires costly nutrients to feed the plants, and also periodic flushing of the systems is required which leads to waste disposal issues.

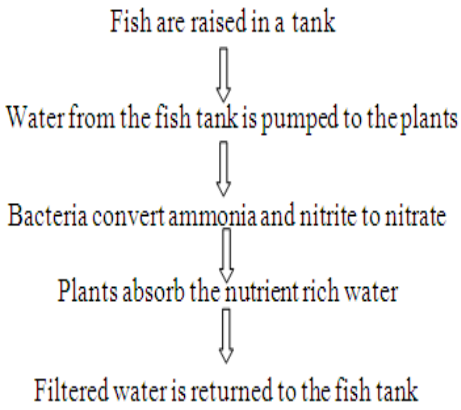
Aquaculture needs to have excess nutrients removed from the system; normally this means that some amount of the water is removed, generally on a daily basis. This nutrient rich water needs to be disposed off regularly and replaced with clean fresh water. While aquaculture and hydroponics are both very efficient methods of producing fish and vegetables, when we look at combining these two, these negative aspects are curved into positives. Fish produces mainly nitrogenous wastes. If these wastes accumulate, it can be fatal for the life of fish, but if they can be managed efficiently then the same waste can be a great fertilizer for plants. As the plants take up these nutrients, they purify the water, which is beneficial for the fish. Many cultures have been made using this cycle to grow better crops and rear the fish as an additional food source. This simple logic is the base for Aquaponics culture. Rice paddies in the China and Thailand and many other countries across the globe have been using aquaponics technique for years. The Aztecs developed a system of building floating islands for food-plants such as maize and squash. Fish use to propagate around the islands, leaving their waste on the lake bottom, where it could be collected to fertilize the plants.

Modern aquaponics is slightly more technically efficient which makes use of environment friendly approach to produce food. Fish are usually kept in large tanks and the plants are grown hydroponically; that is, without soil. Plants are mainly planted in beds with a little gravel or clay and their roots hang down into the water. The water is cycled through the system, so that it collects the "waste" from the fish and recirculates back to the plant beds, where it is naturally filtered by the plants and then again returned to the fish tanks. In this trend of culture, no chemical fertilizers are needed for the plants unlike traditional farming methods as in the present context they all come from the fish-waste. It also tends to be organic, because the use of pesticides would be detrimental to the fish. Thus, aquaponics is a sustainable system that combines both hydroponic (plant) and aquaculture (animal) systems. This system makes use of the natural biological cycles (Nitrification). It allows us to produce fish and plants in a single system with a large reduction in water use (Fig.1)

Why Aquaponics

Aquaponics as an integrated system helps to negotiate many of the crises prevailing across the globe. Some of the common crises are increasing population, food shortages, increasing unemployment, global warming, etc. This system only uses a fraction of the water, about 10% of soil growing. There is no need to purchase, store and apply fertilizer, no soil-borne diseases, no tilling, and no weeds. It results in high fish stocking density, high crop yield. This integrated system relies on the principle of no waste as waste from fish is been used by plants. In other words waste from fish is used to feed the plants. Water is re-used in the re-circulating system. No pesticides or herbicides required rather continuous organic fertilizer is supplied naturally. This system aids to food security as we can grow our own food within a defined space, year-round and equally potent in draught or places with poor soil quality which results in local food production, enhances the local economy and reduces food transportation. Thus, aquaponics is considered as sustainable as it has lots of advantages with respect to hydroponics and aquaculture (Table 1) along with a cutting edge for meeting several crises.

How Aquaponics Works (Fig. 2)



Components

Aquaponics is comprised of two main parts, aquaculture part for raising aquatic animals and the hydroponics part for growing plants (Rakocy, Diver, 2006). Although consisting primarily of these two parts, aquaponics systems are usually catagorized into several components or subsystems responsible for the effective removal of solid wastes, for adding bases to neutralize acids, or for maintaining water oxygenation (Rakocy, 2006). Typical components include:

- Fish Tank
- Place to Grow Plants
- Water Pump(s)
- Air Pump
- Irrigation Tubing
- Water Heater (Optional)
- Filtration (Optional)
- Grow light (Optional)
- Fish and Plants
- Sump
- Settling basin

Fish tank is used to rear fish. Water pumps and air pump are used to regulate the water level and air level respectively. Irrigation tubing is well connected throughout, so that it creates a re-circulating system. Sump is the lowest point in the system where the water flows to and from which it is pumped back to the fish tanks. Settling basin is a unit for catching uneaten food and detached biofilms, and for settling out fine particulates (Fig. 3)

Plants: Hydroponics

Plants are grown as in hydroponics systems, with their roots immersed in the nutrient-rich effluent water. This enables them to filter out the ammonia that is toxic to the aquatic animals, or its metabolites. After the water has passed through the hydroponic subsystem, it is cleaned and oxygenated, and can return to the aquaculture vessels. This cycle is continuous. Without plants the system cannot function properly. Growing plants in soil is fairly easy but takes up valuable space because of moisture and spacing requirements. Aquaponics takes care of this automatically, without much thought except to insure the flow of water. If the electricity quits or a pump fails the plants will survive several days up to two weeks depending on the temperature, but of course the fish will die within hours. Even plants needing large amounts of nitrogen, like tomatoes, can exist side by side with plants that require

little, like lettuce. The nutrient rich water reaches all plants and because it only passes through, only what is needed is used. Even with good plant coverage there are a lot of nitrates flowing out the drains back to the fish tank, enough in fact to power up another group of grow beds. This is not a concern unless the water is cloudy in the fish tank.
Vegetables like Lettuce, Beans, Squash, Zucchini, Broccoli, Peppers, Cucumbers, Peas, Spinach,,etc. **Herbs** like Basil, Thyme, Cilantro, Sage, Lemongrass, Wheatgrass, Oregano, Parsley, etc. **Fruits** like Strawberries, Watermelon, Cantaloupe, Tomatoes, etc. Most garden varieties flowers can also be grown.

Why do Plants like Aquaponics?

- Nutrients constantly provided
- Warm water bathing the roots
- Don't have to search for water or food
- Less effort needed in putting out roots
- All the energy goes into growing UP not DOWN
- No weed competition

All of the above mentioned factors aids all the necessary ingredients responsible for a better and healthy growth of the plants.

What influences the amount of available nutrients to plants?

Many factors as mentioned below held responsible for the availability of nutrients to the plants. These factors should be tightly and timely regulated for the optimum growth of the plants.

- Density of fish population
- Size of fish
- Temperature of water
- Amount of uneaten fish feed in water
- Availability of beneficial bacteria
- Amount of plants in the system
- Media present in system
- Water flow rate

Economical Rising Effectiveness with Vegetables Production

Aquaponics presents an promising opportunity to rethink the traditional fish farming, to fetch in more money at the farm gate. Two profit centers for producers: fish and plants. If fish goes through a stumpy cycle then we have plant revenue to rely on and vice versa. Many experts claim that aquaponics has the potential to produce more than conventional or hydroponics where as some claim it produces considerably less. The integration of fish and plants is a kind of polyculture that increases diversity and thereby enhances system stability. Aquaponics increase economical efficiency because several key costs such as nutrients, land and water are substantially reduced and module operating and infrastructural costs are shared.

The system involves no control of root pathogens, as these are controlled biologically by the broad spectrum of antagonistic micro-organisms that develop in the natural environment (Nichols M, 2008). Aquaponics is a bio-integrated system that associates recirculating aquaculture with hydroponic vegetable, flower, or herb production (Gordon A Chalmers, 2004). This production type of fish and vegetables, is right where the market is headed-consumers are demanding safe food produced in an environmentally responsible way. The fact that aquaponic products are locally produced, and therefore, "leaving a small footprint on earth, is an added bonus". Terms such as "natural", "environmentally friendly", "pesticide free", "organic" have growing attraction to consumers(Graham L, 2003).

Aquaponics process, gives big advantages in earlier and faster plant crop production to capture more profits. This type of agriculture might mean a stepped-up investment, but it is one that creates another revenue stream (from fish) linked with more profitable plant production. Some benefits of this system outlined by Amadis Lacheta (2010):

- Faster growth rate, crop maturity and yields
- Consistency and quality of crops
- Drastically reduced water and nutrients compared with soil-grown produce
- Crops can be grown in places where ordinary horticulture and aquaculture is impossible due to poor or contaminated soil or water
- Reduced growing area required
- Systems can be set up at a comfortable working height, excellent for people who are elderly or have disabilities
- Relative freedom from soil diseases and pests
- Weeds are virtually non-existent
- Water stress is reduced in hot conditions
- Less ongoing maintenance required

Increasing economical efficiency of aquaculture by aquaponics, is given from the fact that by this innovation water consume is reduced to minimum and most important we obtain organic vegetable products, that means an additional product which brings to us extra cash.

Animals: Aquaculture

Aquariums require filtering systems that must be either cleaned or replaced on a regular basis. The grow beds of the aquaponics system by themselves act as this filter without the hassle of cleaning or replacing. Of course, plants must be present in the grow beds. Almost many freshwater fish can be raised in the system although the operating temperature may prohibit rearing of some species such as trout. Freshwater fish are the most common aquatic animal raised using aquaponics, Fish like aquarium fish, Tilapia, Trout, Catfish, Yellow Perch, Bass, Bluegill, Carp, Koi, Goldfish, freshwater Prawns are recommended for rearing in an aquaponic system.

Fish Maintenance

- Feed fish 2 - 3 times a day, but shouldn't be overfed
- Fish eat 1.5 – 2% their body weight per day, this should be taken care of
- Fish should be feeded only that which they can eat in 5-10 minutes
- Fish won't eat if they are too cold, too hot or stressed, thus temperature conditions should be well regulated
- Water quality should be checked periodically
- Fish behaviour and appearance should be observed

Fish Health Management

- Good hygiene and bio security—prevention, avoidance, selective access, and commonsense should always be exercised.
- Before stocking fish from other facilities into own's system it should be quarantined properly. Their health should be monitored for several days—treat if necessary.
- The best defense is fish's own immune system. Always there should be a low-stress environment so that fish will maintain their health.

Bacteria

Nitrification which involves the aerobic conversion of ammonia into nitrates, is one of the most important functions in an aquaponics system as it helps in reducing the toxicity of the water for fish, and thus allows the resulting nitrate compounds to be removed by the plants for nourishment (Rakocy, 2006). Ammonia is steadily released into the

water through the excreta and gills of fish as a product of their metabolism, but must be filtered out of the water as higher concentration is detrimental to fish. Although plants can absorb ammonia from the water to some degree, nitrates are assimilated more easily thereby efficiently reducing the toxicity of the water for fish (Rakocy, 2006). Ammonia can be converted into other nitrogenous compounds through:

- *Nitrosomonas*: bacteria that convert ammonia into nitrites, and
- *Nitrobacter*: bacteria that convert nitrites into nitrates.

In an aquaponics system, the bacteria responsible for this process form a biofilm on all solid surfaces throughout the system that are in constant contact with the water. The submerged roots of the vegetables combined have a large surface area, so that many bacteria can accumulate there. Care for these bacterial colonies is important as to regulate the full assimilation of ammonia and nitrite. This is why most aquaponics systems include a biofiltering unit, which helps facilitate growth of these microorganisms. Since the nitrification process acidifies the water, non-sodium bases such as potassium hydroxide or calcium hydroxide can be added for neutralizing the water's pH. In addition, selected minerals or nutrients such as iron can be added in addition to the fish waste that serves as the main source of nutrients to plants (Rakocy, 2006).

A good way to deal with solids buildup in aquaponics is the use of worms, which liquefy the solid organic matter so that it can be utilized by the plants and/or animals.

Technical Operation

Ten key guiding principles for creating successful aquaponics systems were issued by Dr. James Rakocy, the director of the aquaponics research team at the University Of The Virgin Islands, based on extensive research done as part of the *Agricultural Experiment Station* aquaculture program:

- Use a feeding rate ratio for design calculations
- Keep feed input relatively constant
- Supplement with calcium, potassium and iron
- Ensure good aeration
- Remove solids
- Be careful with aggregates
- Oversize pipes
- Use biological pest control
- Ensure adequate biofiltration
- Control pH

The vital inputs to the system are water, oxygen, light, feed given to the aquatic animals, etc. In terms of output, an aquaponics system may frequently yield plants such as vegetables grown in hydroponics, and edible aquatic species raised in an aquaculture. Typical build ratios are .5 to 1 square foot of grow space for every 3.8 L of aquaculture water in the system. 3.8 L of water can support between 0.23 kg and 0.45 kg of fish stock depending on aeration and filtration. Target pH should be maintained between 7.0 – 8.0. A thorough knowledge of the organisms in the system is required for success. pH, ammonia, dissolved Oxygen, soluble Salts, alkalinity, nitrate are some of the measures for water quality which should be monitored periodically.

Safe Materials

All the components used in the system should be made sure that they are safe for fish and humans:

- Polypropylene - labeled PP
- High Density Polyethylene - labeled HDPE
- High Impact ABS (Hydroponic Grow Trays)
- Stainless Steel barrels
- EPDM or PVC (poly vinyl chloride) pond liner (make sure its UV resistant and avoid fire retardant material)
- Fibreglass tanks and grow beds

- Rigid white PVC pipe and fittings, black flexible PVC tubing, some ABS
- DO NOT use Copper – Its toxic to the fish

System Maintenance

- Fish should be feeded daily and their health should be monitored regularly.
- Water quality should be tested (every other day for the first month, then about once a week, then as needed).
- Filter screens, filter tanks (if using), tubing, water pump, growbed media, etc. should be cleaned out as and when needed.
- Plant health should be checked.
- Plants should be checked for bugs or nutrient deficiencies in a regular fashion.

System Start-up Checklist

- Type and size of system to build should be clearly decided
- Drawing to be done for designs, research where to get parts, plan
- Components should be brought and assembled properly
- Plants should be grown from seed or some source for seedlings should be found
- System should be filled with water and circulated (at least a week)
- About 20% of stocking density of fish should be added to the system
- Water quality should be monitored and partial water changes should be done as and when needed
- System should be maintained properly

Handy Tips and Tricks

- Gravel media should be washed before putting into the system – otherwise it will lead to very cloudy dirty water
- pH of the gravel media should be tested
- Vitamin C and an air pump to bubble out chlorine and chloramines from tap water should be used
- Worms (red wigglers) need to be used in media beds to breakdown solids and reduce anaerobic zones
- Cleaning products, pesticides, algaecides, fertilizers or like substances shouldn't be used in fish tanks or grow beds
- Plants should be sprayed with diluted vinegar and water solution if aphides infects the plants
- Direct sunlight on fish tanks should be avoided, the top should be covered to avoid algae and make fish happy
- More than 1/3 of water at a time shouldn't be changed. More than that will destroy the good bacteria in the system.
- Outdoor plants should be covered during a frost, and shade from the scorching summer sun. We need to make sure that we have backup power available for pumps and aerators

Benefits from Aquaponics

- **Addresses issues on food safety**
  – Produce do not contain the most common pathogen
- **Maximizes the use of space**
  – Diversified operations (fish and plants)
  – Ability to produce a large quantity of food in a small space
  – No land is needed
- **Ease of operation**
  – No weeding
  – No soil cultivation
  – Minimal watering
  – No pesticide application

– Minimal maintenance and time spent
- **Addresses issues on climate change**
  – Conserves water
  – No leaching of nutrients or waste to be pumped into the environment
- **A great educational tool to teach children grows food and care for living things**
- **Operation is friendly to persons with physical disability**
- **Products are higher in nutrient and better**

Future Perspectives

Simplicity in design and management with almost no energy and low equipment costs makes these systems an interesting solution wherever land availability, flooding, productivity and ecological footprint are an major issue. In addition the employ of water weeds as a resource can certainly increase livelihoods opportunities in all those areas affected worldwide. Further research needs to address the nutrient dynamics of different growing media and to optimise system design and nutritional requirement of vegetables in those water bodies with limited dissolved nutrients. The possibilities of this integrated system are quite high and can provide sensitive benefits to smallholders as well as big aquaculture enterprises. The potential of these systems is however not fully understood and interdisciplinary links and research can unquestionably address many of the issues that are still hidden.

CONCLUSION

Aquaponics is the combination of aquaculture and hydroponic systems whereby nutrient rich waste water from the aquaculture system is engaged into the hydroponic system. The trends of new millennium in environmental regulation, are limiting amount of water which may be consumed or discharged. In aquaponics, wastewater from aquaculture is filtered and is recirculated into the system. Aquaponics presents an opportunity to rethink the traditional fish farming, to bring in more money farm gate.

“The ultimate goal of farming is not the growing of crops, but the cultivation and perfection of human beings.” — Masanobu Fukuoka, the One-Straw Revolution

Author Contribution Statement

Gagan Kumar Panigrahi and Annapurna Sahoo conceived the idea. All authors contributed significantly in drafting the manuscript.

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Conflict of Interest

The authors declare that they have no conflict of interest.

REFERENCES

1. Diver S, 2006. Aquaponics—Integration of Hydroponics with Aquaculture (Internet). ATTRA - National Sustainable Agriculture Information Service. Available from: <http://attra.ncat.org/attra-pub/PDF/aquaponic.pdf> (accessedon 02/4/2008)
2. Duong Tan Nhut , Nguyen Hoang Nguyen, Dang Thi Thu Thuy, "A novel in vitro hydroponic culture system for potato (Solanum tuberosum L.) microtuber production", ScienceDirect ,2006.
3. Gordon A Chalmers, "Aquaponics and Food Safety", Lethbridge, Alberta April, 2004.
4. Hutchinson, W, Jeffrey, M, O'Sullivan, D., Casement, D. , Clarke, S., " Recirculating Aquaculture Systems: Minimum Standards for Design, Constructionand Management.", Inland Aquaculture Association of South Australia Inc. , 2004.
5. Jensen, M.H., "Hydroponics.", HortScience, 32(6):1018–1021. 1997.
6. Malcolm, J. , "What is aquaponics?", Backyard Aquaponics, Issue 1, Summer 2007.
7. Nichols M, "Aquaponics: Where One Plus One Equals Three
8. ", Massey University, Palmerston North, New zeeland, Maximum Yeld- Indoor gradening, UK January-February 2008
9. Pantanella, E., "Pond aquaponics: new pathways to sustainable integrated aquaculture and agriculture", Aquaculture News, May 2008
10. Rakocy, James E.; Masser, Michael P.; Losordo, Thomas M. (November 2006). *Recirculating aquaculture tank production systems: Aquaponics — integrating fish and plant culture* (454). Southern Regional Aquaculture Center.

Table 1: Comparison between hydroponics, aquaculture and aquaponics.

System	Advantages	Disadvantages
Hydroponics	• Produces a high volume of crops in a small space • The most water efficient method of crop production	• Dependent on manufactured fertilizers that are costly
Aquaculture	• Produce a large volume of fish in a small space	• It has a high rate of failure due to high stocking rates • Fish produce ammonia, algae, minerals that are to be constantly filtered
Aquaponics	• No pesticide, thereby reducing carbon footprint • The plants get an automatic food supply from the fish water • The plants filter the water for the fish	• Management requires skills in growing fish and plants

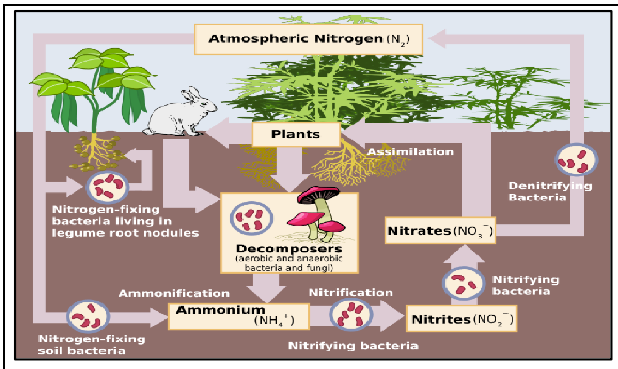

Fig.1 Aquaponics basic diagram

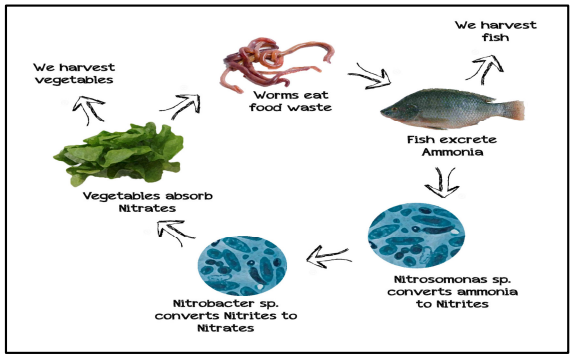

Fig. 2 Diagram illustrating general working of Aquaponics

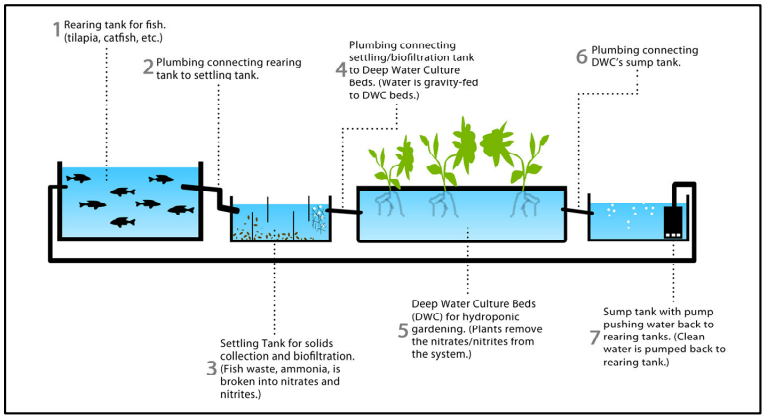

Fig. 3 General setup of an aquaponics system

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RESEARCH ARTICLE

Determination of Limnological Parameters That Affects the Fish Productivity

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ABSTRACT

Physical,chemical and biological parameters like Temperature, Total alkalinity, pH, Dissolved oxygen, Nitrate Nitrogen and planktons were studied in three ponds (1,2 & 3) in Khurda district of Odisha. The parameters studied in all the ponds varied but statistically insignificant. The ponds were stabilized empowering the people with the techniques for composite fish farming using *Catla, Rohu* and *Mrigal* as candidates for harvesting.

Keywords: Temperature, total alkalinity, planktons, ponds.

INTRODUCTION

Limnology is defined as the study of fresh water andtheir inhabitants. The growth and survival of aquaticinhabitants depend on the quality of water Boyd 1989,1990, Philips 1991, Jhingran 1985. The quality of water depends on the physical, chemical and biologicalcharacteristics of water is known.Zweig et al. 1999, Adeniji and Ovie 1982; Das and Padhi2014,Padhi et al. 2015. Hence the present study isfocussed on the determination of quality of water in order toutilize the ponds for aquaculture.Fish plays an important role in agriculture sector ofIndia. It provides livelihood to more than 60 million peopleand earns more than 6800 crore rupees through export. Limnological studies have been carried out by Olopade 2013 and Nikolosky 1963.The Main objectives of the study was to determinephysical, Chemical and biological characteristics of pondsin order to utilize them for fish culture and thus generateemployment opportunity for gainful earning among ruralpeople by creating awareness among them

through trainingon aquaculture practices.Composite fish farming is the technique to culture different types of compatible and non competitive fishes in the same ecosystem so as to allow them to grow by feeding by making optimum use of different zones (surface,bottom and column) of the ponds without impeding the growth,development and maturity of one another.This is a very profitable method of aquaculture and hence importance has been laid to train the populace for gainful employment.

MATERIALS AND METHODS

For the purpose of study, three ponds in three villages (Khudpur, Podopoda, and Barapada) in Khurda district, Odisha, were chosen for investigation, and such ponds were not utilized for fish cultivation earlier. The parameters chosen were water temperature, P^H, dissolved oxygen, total alkalinity, nitrate nitrogen and plankton biomass of water.Temperature was recorded using ordinarythermometer (accurate up to 0.01 degree C), $P^H$by P^H meter, alkalinityby using phenopthalein and methyl orange indicaters. Dissolved oxygen was measured by Wrinkler'smethodand nitrate nitrogen and plankton biomass were measured byfollowing standard procedures (APHA-2005) using watertesting kits (NICE). During the period from November 2018to October 2019.

Preparation of Ponds for Composite Fish Culture

a)Cleaned the ponds by making free from undesirable plants and weeds manually.
b)Liming the ponds was done in order to correct the acidity of soil and water to speed up the decomposition of organic matter; which acts as disinfectant and as an essential nutrient (@ 200 kg/ha).
c) Fertilizing the ponds was done after 3 days of liming for bloom of phytoplankton and growth of zoo plankton by manuring with organic manures (cowdung and oil cake @ 500 kg/ha) which carry almostall nutrients required by fish.The inorganic manures like urea @ 60 kg/ha/month and single super phosphate @ 70 kg/ha/month were used depending on the soil and water condition of the different ponds as they provide the nutrients, vitamins and minerals to the fish thus increasing natural productivity of the ponds.
d)Artificial feeding was done by providing rice bran, oil cake and kitchen waste as these are cheaply available.
e) After cleaning, liming and fertilizing the ponds during March-April 2013, the fingerlings of 50-100 gm size (approx) purchased from govt.hatcheries were stocked in the ponds 15 days after fertilization of ponds. Fingerlings of *Catla*, *Rohu*amd*Mrigal* in the ratio of 4:3:3 wereselected to get good yield in mixed farming during July2013.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth Gupta and Gupta 2006.The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality Zweig et al. 1999.Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment.The results (Fig.1-5) indicate that the water temperature in pond 1 varied from 19 to 32, in pond 2 from 19.3 to 33.5 and in pond 3 from 21 to 33.1. pHin pond 1 varied from 7.4 to 8.1, in pond 2 from 7.5 to 8.2 and in pond 3 from 7.4 to 8.1. Total alkalinity showed 81.3 to 184.86 in pond 1, from 86.20 to 196.15 in pond 3 and varied from 84.18 to 196.24.Dissolved oxygen values varied from 5.4 to 8.5 in pond 1, from 5.5 to 8.3 in pond 2 and from 5.6 to 8.1 in pond 3.Nitrate nitrogen varied from 0.98 to 5.28 in pond 1, from 0.96 to 8.21 in pond 2 and from 2.38 to 15.35 in pond 3.Phytoplankton analysis revealed variation from 212 to 218 in pond 1, 224 to 231 in pond 2 and 225 to 238 in pond 3.Zooplankton varied from 20 to 38 in pond 1, 27 to 35 in pond 2 and from 26 to 31 in pond 3 during different months of the year (2018-2019) under study. Taking all these factors into consideration, the three ponds under study were prepared for fish culture by cleaning, liming, fertilizing, stocking and artificial feeding for harvesting after one year.The result (range of variation of different parameters)obtained on three ponds (P1, P2, P3, Average Depth of 3.5-5')during the period of study(Nov 2018 to Oct 2019), were recorded. After having studied, the pond health, treatment

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CONCLUSION

Catlacatla(surface feeder) *Labeorohita*(column feeder)and *Cirrhinamrigala*(bottom feeder) and with differentfeeding habits occupying different zones of the ponds utilizethe available food of the ponds in all the zones profitably.Regularly the weeds were removed by physicalmethods, manuring was done alongwithproviding artificial diet like oil cakes,waste vegetables etc.,the fish were caught and weighed at intervals. The fish werecaught by netting during March-April 2013. The weight offish, ranged from 500gm-1000gm. Fishes below 500gm wereagain left in the ponds for further growth.The average yield of fishes and their cost at site was from P1-250kg, from P2-253kg and from P3-255kg @ Rs 100/kg and the total sale price was Rs. 82,800 in the year under study.Awareness programmes were organized periodicallyin the villages in order to create awareness among people inorder to motivate them for fish cultivation. The resourcepersons were invited from Fishery Training Institute,Balugaon; WBUAFS, Kolkata; Berhampur University andfrom CIFA, Bhubaneswar.Training programmes on composite fish farmingwere organized forVillagers and students. The technical expertise so gained isbelieved to be utilized by the beneficiaries for gainful earning.During the period of study care of the ponds was monitored by a group of peer volunteers from each village who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of fish was being used as seed money by the volunteersfor cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

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REFERENCES

1. Adeniji, H.A. and Ovie, S.I. 1982. Study and appraisal for the water quality of the AseOli and Niger Rivers. NIFFER Annual Report, 15-20.
2. APHA. 2005. Standard methods for examination for water and waste water, 17th edition. American Public Health Association. Washington DC.

3. Boyd, C.E. 1989. Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham AlaAubum University Press.
4. Boyd, C.E. 1990. Water quality in ponds for aquaculture. Albama agricultural experiment station, Auburn University Ala.
5. Das, S.K. and Padhi, S.N. 2014. In Application of Biology for Self Employment. Ed. Vol. Nanda Kishore Publication, Bhubaneswar.
6. EPA, 2006. "Water Quality Standards Review and Revision, Washington DC.
7. Gupta, S.K. and Gupta, P.C. 2006. General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
8. Jhingram, V.G. 1985. Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
9. Nikolosky, G.V. 1963. The ecology of fishes. Academic Press, London, U.K.
10. Olopade, daniyi 2013. Lakes reservoirs and ponds. 7 (1), 9-19.
11. Padhi, S.N., Das, S.K.,Panda, A. and Panda, Sasmita. 2015. In Employment through aquaculture. Nanda Kishore Publication, Bhubaneswar.
12. Philips, M.J., Beveridge, M.C.M. and Clark R.M. 1991. Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture Vol.3:568-591.
13. Zweig, R.D., Morton, J.D. and Stewart, M.M. 1999. Source water quality for aquaculture. A guide for assessment World Bank Report, 74.

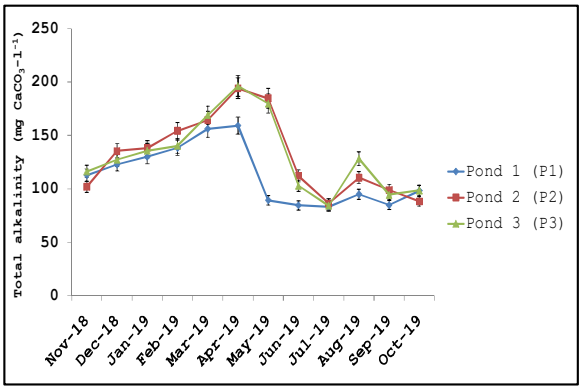

Fig. 1: Variations in total alkalinity (mg CaCO3-l^{-1}) in different ponds (Nov 2018-Oct-2019)

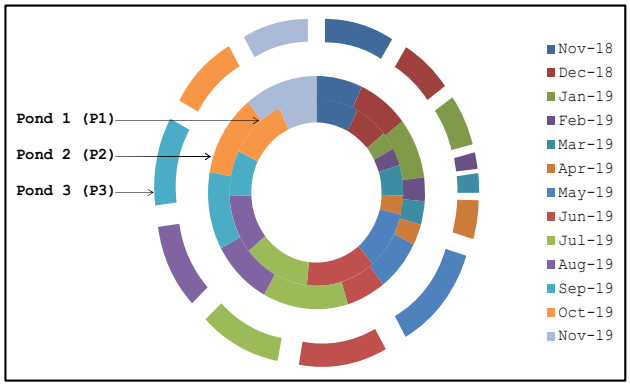

Fig. 2: Variations of nitrate-nitrogen (µg-l^{-1}) in different ponds (Nov 2018-Oct-2019).

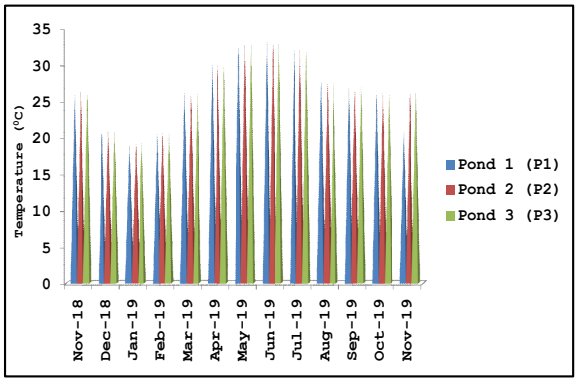

Fig.3: Temp. (^{0}C) in three ponds (Average value) (Nov 2018-Oct-2019).

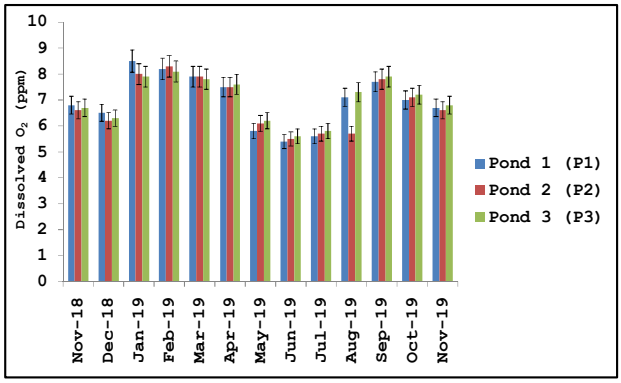

Fig.4: Dissolved oxygen (DO) in three ponds (in ppm) (Nov 2018-Oct-2019).

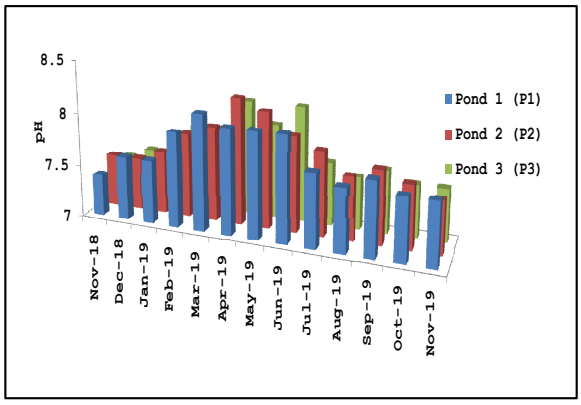

Fig.5: pH in three ponds (Average value) (Nov 2018-Oct-2019).

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RESEARCH ARTICLE

Effect of Limnological Characteristics of Ponds on Composite Fish Culture for Improvement of Livelihood of Fisherman

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ABSTRACT

This study deals with the ecology of temporary ponds in the east coast of India from November 2018 to July 2019. Three categories of ponds were recognized on the basis of physical and biotal characteristics. Each of the ponds displayed a detritus-based food web derived predominantly from leaf litter. Productivity in all the ponds was contributed due to aquatic vegetations and phytoplankton. Physico-chemical parameters including physical, chemical and biological parameters like temperature, total alkalinity, pH, dissolved oxygen, nitrate and nitrogen contents of the pond water were investigated. There was no consistent pattern across the ponds, though community metabolism reports showed that the ponds which are exposed are autotrophic whereas the shaded ponds are heterotrophic in nature. Most importantly, the ponds were stabilized empowering the people with the techniques for composite fish farming of Indian major carps (*Catla catla, Labeo rohita* and *Cirrhinusmrigal*) as candidates for harvesting. The present investigation was carried out on certain water quality and biotic parameters of a fish pond in different time intervals. The pH found to be between 7.4 and 8.2. The total alkalinity ranged between 130 to 218(mg $CaCO_3.l^{-1}$).The water quality of the pond was moderate for aquatic organism and fishes.

Keywords: Physico-chemical, limnology, water, fish, alkalinity, ponds.

INTRODUCTION

Ecosystem is predominantly the basic and fundamental unit of ecology. It provides information regarding the availability of solar energy in a habitat and also about the accessibility of mineral elements, their utilization and recycling. Majorly, the microorganisms, plants and animal present in an ecosystem makeup the biotic component whereas the physical and chemical components/factors represent the abiotic components of an ecosystem. Water resources are continuously deteriorating everyday at a quicker rate primarily due to hasty population and urbanization load. Declining water quality is currently a global issue (Mahananda et al., 2010). The water purity varies from place to place in nature (Patil 2013). Essentially, the interaction between physical, chemical and biological components of a habitat determines the quality of water of an ecosystem. Mostly, aquatic biota influences the physico-chemical characteristics of an aquatic ecosystem (Sharma et al., 2009).

Limnology essentially deals with the study of fresh water andtheir inhabitants. Primarily, the growth and survival of fresh waterinhabitants depend on the quality of water(Boyd, 1989; Boyd, 1990; Philips, 1991; Jhingran, 1985). Fish plays an important role in agriculture sector of India. It provides livelihood to more than 60 million people and earns more than 6800 crore rupees through export. Extensive limnological studies have been carried out (Olopade, 2013; Nikolosky, 1963). The quality of water predominantly depends on the physical, chemical and biologicalcharacteristics of water (Zweig et al. 1999; Adeniji and Ovie 1982; Das and Padhi,2014; Padhi et al. 2015). Mostly, the present study isfocused on the determination of quality of water in order toutilize the ponds for aquaculture.The Main objectives of the study was to determinephysical, chemical and biological characteristics of pondsin order to utilize them for fish culture and thus generateemployment opportunity for gainful earning among ruralpeople by creating awareness among them through trainingon aquaculture practices.Composite fish farming is the technique to culture different types of compatible and non competitive fishes in the same ecosystem so as to allow them to grow by feeding by making optimum use of different zones (surface,bottom and column) of the ponds without impeding the growth,development and maturity of one another.This is a very profitable method of aquaculture and hence importance has been laid to train the populace for gainful employment.

MATERIALS AND METHODS

Study Site

For the purpose of study, three ponds (P1, P2 and P3) in three villages in the state of Odisha, India were chosen for investigation, and such ponds were not utilized for fish cultivation earlier.

Measuring Physico-Chemical Parameters

The parameters chosen were water temperature, pH, dissolved poxygen, total alkalinity, nitrate nitrogen and plankton biomass of water.Temperature was recorded using thermometer (accurate up to 0.01 degree Celsius), pHbypH meter, and alkalinityby using phenolphthalein and methyl orange indicators. Dissolved oxygen was measured by Wrinkler's methodand nitrate nitrogen were measured byfollowing standard procedures (APHA-2005) using watertesting kits (NICE), during the period from November 2018to October 2019.

Preparation of Ponds for Composite Fish Culture

The ponds were manually cleaned by making free from undesirable plants and weeds manually.Liming of the ponds was done in order to modulate the acidity of soil and water to speed up the decomposition of organic matter; which acts as disinfectant and also as an essential nutrient. Fertilizing the ponds was done after 3 days of liming for bloom of phytoplankton and growth of zoo plankton by manuring with organic manures like cowdung and oil cake (500 kg/ha) which carry almostall nutrients required for fish growth.

Fish Feeding

The inorganic manures like urea (60 kg/ha/month) and single super phosphate (70 kg/ha/month) were used depending on the soil and water condition of the different ponds as they provide the nutrients, vitamins and minerals to the fish thus increasing natural productivity of the ponds.Artificial feeding was done by providing rice bran, oil cake and kitchen waste as these are cheaply available.

Introducing Fingerlings in the Pond

After cleaning, liming and fertilizing the ponds during March-April 2018, the fingerlings of 50-100 gm size (approx) purchased from govt.hatcheries were stocked in the ponds 15 days after fertilization of ponds. Fingerlings of *Catla, Rohu* amd *Mrigal* in the ratio of 4:3:3 wereselected to get good yield in mixed farming during July2018.

Statistical Analysis

Each experiment was done in triplicates to validate the significance of the results.

RESULTS AND DISCUSSION

The maintenance of good water quality is essential for both survival and optimum growth (Gupta and Gupta 2006). The water quality standards vary significantly due to different environmental conditions, ecosystem and intended human users EPA 2006. The quality of aquaculture products and their suitability for human consumption may also be affected by water quality (Zweig et al. 1999).Keeping these factors in view, the ponds under study were maintained for aquaculture imparting training to local people also in order to empower them for gainful employment.The results (Table I-V, Fig 1-5) indicate that the water temperature in pond 1 varied from 19 to 32, in pond 2 from 19.3 to 33.5 and in pond 3 from 21 to 33.1. pHin pond 1 varied from 7.4 to 8.1, in pond 2 from 7.5 to 8.2 and in pond 3 from 7.4 to 8.1. Total alkalinity showed 81.3 to 184.86 in pond 1, from 86.20 to 196.15 in pond 3 and varied from 84.18 to 196.24.Dissolved oxygen values varied from 5.4 to 8.5 in pond 1, from 5.5 to 8.3 in pond 2 and from 5.6 to 8.1 in pond 3.Nitrate nitrogen varied from 0.98 to 5.28 in pond 1, from 0.96 to 8.21 in pond 2 and from 2.38 to 15.35 in pond 3.Phytoplankton analysis revealed variation from 212 to 218 in pond 1, 224 to 231 in pond 2 and 225 to 238 in pond 3.Zooplankton varied from 20 to 38 in pond 1, 27 to 35 in pond 2 and from 26 to 31 in pond 3 during different months of the year (2018-2019) under study. Taking all these factors into consideration, the three ponds under study were prepared for fish culture by cleaning, liming, fertilizing, stocking and artificial feeding for harvesting after one year.The result (range of variation of different parameters)obtained on three ponds (P1, P2, P3, Average Depth of 3.5-5')during the period of study(Nov 2018 to Dec2019), were recorded: (Table VI).After having studied, the pond health, treatment was done preparing the ponds for aquaculture following standard prescribed guidelines for pre stocking, stocking and harvesting.

CONCLUSION

Catla catla (surface feeder), *Labeo rohita* (column feeder) and *Cirrhina mrigala* (bottom feeder) and with different feeding habits occupying different zones of the ponds utilize the available food of the ponds in all the zones profitably. Regularly the weeds were removed by physical methods, manuring was done along with providing artificial diet like oil cakes, waste vegetables etc., the fish were caught and weighed at intervals. The fish were caught by netting during March-April 2018. The weight of fish, ranged from 500gm-1000gm. Fishes below 500gm were again left in the ponds for further growth. The average yield of fishes and their cost at site was from p1-280kg, from P2-263kg and from P3-285kg @ Rs 100/kg and the total sale price was Rs. 82,800 in the year under study (2018-2019) (Table VII). Awareness programmes were organized periodically in the villages in order to create awareness among people to motivate them for fish cultivation. Training programmes on composite fish farming were organized for villagers and students. The technical expertise so gained is believed to be utilized by the beneficiaries for gainful earning. During the period of study care of the ponds was monitored by a group of peer volunteers from each village

who have assisted in managerial activity and watch of the ponds in their respective villages. The profit of the sale proceeds of fish was being used as seed money by the volunteers for cultivation of fish for livelihood besides other engagements. Thus the objectives have been achieved through training and interaction sessions generating confidence among the villagers for aquaculture for their livelihood.

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REFERENCES

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3. Boyd, C.E. 1989. Water quality management and aeration in shrimp farming. Fishes and Allied Aquaculture Department Series. No. 2. Birmingham Ala Aubum University Press.
4. Boyd, C.E. 1990. Water quality in ponds for aquaculture. Albama agricultural experiment station, Auburn University Ala.
5. Das, S.K. and Padhi, S.N. 2014. In Application of Biology for Self Employment. Ed. I Vol. 1, Nanda Kishore Publication, Bhubaneswar, India.
6. EPA, 2006. "Water Quality Standards Review and Revision, Washington DC.
7. Gupta, S.K. and Gupta, P.C. 2006. General and applied technology (Fish and Fisheries) S. Chand and Company, New Delhi.
8. Jhingram, V.G. 1985. Fish and fisheries of India. Hindustan Publishing corporation, Delhi, India.
9. Mahananda, M.R., B.P. Mohanty & N.R. Behera 2010. Physico-chemical analysis of surface and ground water of Bargarh District, Orissa, India. Int. J. Res. Rev. Appl. Sci., 2(3): 23-29
10. Nikolosky, G.V. 1963. The ecology of fishes. Academic Press, London, U.K.
11. Olopade, daniyi 2013. Lakes reservoirs and ponds. 7 (1), 9-19.
12. Padhi, S.N., Das, S.K.,Panda, A. and Panda, Sasmita. 2015. In Employment through aquaculture. Nanda Kishore Publication, Bhubaneswar.
13. Patil, A.A. 2013. Status of water quality of Bhambarde and Lengre reservoir of Sangli district, Maharashtra (India). Flora and Fauna, 19(1): 35-40

14. Philips, M.J., Beveridge, M.C.M. and Clark R.M. 1991. Impact of aquaculture on water resourses. In D.E. Brune and J.R. Tomasso (eds), Advance in aquaculture Vol.3:568-591.
15. Sharma, K., K. Shvetambri, P. Verma & S. P. Sharma 2009. Physico-chemical assessment of three freshwater ponds of Jammu (J&K), Curr. World Environ., 4(2): 367-373.
16. Zweig, R.D., Morton, J.D. and Stewart, M.M. 1999. Source water quality for aquaculture. A guide for assessment World Bank Report, 74.

Table I: Variations in total alkanity (mg $CaCO_3.l^{-1}$) in different ponds.

Month/Period		P_1	P_2	P_3
Nov 2018	I	81.36	105.85	112.25
	II	112.72	101.72	116.20
Dec 2018	I	124.58	109.95	120.16
	II	122.78	135.4	127.35
Jan 2019	I	134.26	134.62	120.60
	II	129.85	138.12	135.70
Feb 2019	I	142.18	148.70	128.3
	II	138.26	154.20	140.20
Mar 2019	I	151.34	147.25	156.15
	II	156.10	164.26	168.92
Apr 2019	I	162.96	152.85	178.34
	II	159.14	194.10	196.24
May 2019	I	184.86	196.15	184.12
	II	89.14	184.72	179.80
Jun 2019	I	94.42	110.62	132.40
	II	84.36	112.10	102.80
Jul 2019	I	82.98	105.20	96.20
	II	83.16	86.20	84.18
Aug 2019	I	110.18	108.15	89.10
	II	94.82	110.42	128.12
Sep 2019	I	89.54	95.20	89.25
	II	84.80	98.90	94.36
Oct 2019	I	96.30	94.65	98.12
	II	98.12	88.12	98.40
Nov 2019	I	90.10	92.10	105.20
	II	110.30	112.30	110.15
Dec-19	I	90.8	91.1	104.9
	II	109.6	111.6	108.9

Table II: Variations of nitrate-nitrogen (µg-l^{-1}) in different ponds.

Month/Period		P_1	P_2	P_3
Nov 2018	I	2.89	10.96	9.18
	II	3.20	4.38	10.95
Dec 2018	I	2.98	5.32	9.40
	II	2.56	4.96	8.36
Jan 2019	I	2.10	6.75	8.52

	II	1.26	5.32	7.48
Feb 2019	I	0.98	4.26	5.10
	II	1.26	2.10	2.38
Mar 2019	I	1.32	1.26	2.56
	II	2.15	2.09	2.86
Apr 2019	I	1.18	0.96	3.94
	II	1.35	1.85	5.69
May 2019	I	2.12	1.23	7.20
	II	4.10	4.56	15.35
Jun 2019	I	4.34	5.38	14.18
	II	5.28	3.75	13.92
Jul 2019	I	4.96	6.14	14.16
	II	5.10	8.10	12.89
Aug 2019	I	3.63	6.45	14.36
	II	4.12	5.82	12.40
Sep 2019	I	3.96	5.10	15.10
	II	3.24	6.89	12.96
Oct 2019	I	4.10	8.21	10.85
	II	4.36	7.26	11.10
Nov 2019	I	3.52	7.10	9.95
	II	2.87	6.95	10.42
Dec 2019	I	3.30	6.91	9.56
	II	2.64	6.60	9.36

Table III: Temp. (in ^{0}C) in three ponds (Average value).

Month/Period	P_1	P_2	P_3
Nov 2018	26	26.4	26.5
Dec 2018	20.8	21.1	21
Jan 2019	19	19.3	19.2
Feb 2019	20.5	20.8	20.6
Mar 2019	26.1	26	26.1
Apr 2019	30.2	30	30.1
May 2019	33	33.1	33
Jun 2019	33.3	33.5	33.1
Jul 2019	32	32.1	32.1
Aug 2019	28	27.6	27.6
Sep 2019	27	26.8	27
Oct 2019	26.3	26.1	26.1
Nov 2019	20.8	26.5	26.4
Dec 2019	21.32	22.46	21.31

Table IV: Dissolved oxygen (DO) in three ponds (in ppm).

Month/Period	P_1	P_2	P_3
Nov 2018	6.8	6.6	6.7
Dec 2018	6.5	6.2	6.3
Jan 2019	8.5	8.0	7.9
Feb 2019	8.2	8.3	8.1
Mar 2019	7.9	7.9	7.8
Apr 2019	7.5	7.5	7.6
May 2019	5.8	6.1	6.2
Jun 2019	5.4	5.5	5.6
Jul 2019	5.6	5.7	5.8
Aug 2019	7.1	5.7	7.3
Sep 2019	7.7	7.8	7.9
Oct 2019	7.0	7.1	7.2
Nov 2019	6.7	6.6	6.8
Dec 2019	6.9	6.8	6.7

Table V: pH in three ponds (Average value)

Month/Period	P_1	P_2	P_3
Nov 2018	7.4	7.5	7.4
Dec 2018	7.6	7.5	7.5
Jan 2019	7.6	7.6	7.4
Feb 2019	7.9	7.8	7.8
Mar 2019	8.1	7.9	7.8
Apr 2019	8.0	8.2	8.1
May 2019	8.0	8.1	7.9
Jun 2019	8.0	7.9	8.1
Jul 2019	7.7	7.8	7.6
Aug 2019	7.6	7.6	7.5
Sep 2019	7.7	7.7	7.6
Oct 2019	7.6	7.6	7.5
Nov 2019	7.6	7.5	7.5
Dec 2019	7.5	7.5	7.5

TableVI: Range of variation of Parameters (November 2018 to October 2019)

Parameters	P1	P2	P3
Temperature	19-32	19.3-33.5	21-33.1
Total alkalinity	81.36-184.86	86.20-196.15	84.18-196.24
pH	7.4-8.1	7.5-8.2	7.4-8.1
Dissolved Oxygen	5.4-8.5	5.5-8.3	5.6-8.1
Phyto plankton (no/lit)	212-218	224-231	225-238
Zoo plankton (no/lit)	20-38	27-35	26-31
Nitrate nitrogen	0.98-5.28	0.96-8.21	2.38-15.35

Table VII: Post-harvestment output

Species	P1(3500Sq.ft)	P2(3600 Sq.ft)	P3(4000Sq.ft)
Catla catla	102 KG	118kg	130kg
Labeo rohita	98kg	75kg	85kg
Cirrhinus mrigala	80kg	70kg	70kg
Total yield	280kg	263kg	285kg
Sale price	28,000	26,300	28,500
Approx expenditure	10,000	10,000	10,000
Profit (Indian rupaiya)	18,000	16,300	18,500

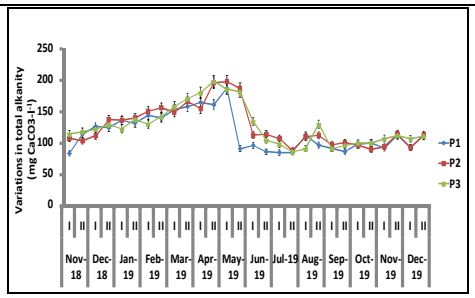

Fig 1. Variations in total alkalinity in different ponds (Nov, 2018-Dec, 2019)

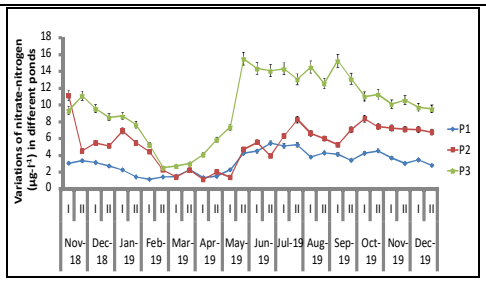

Fig 2. Variations of nitrate-nitrogen in different ponds (Nov, 2018-Dec, 2019)

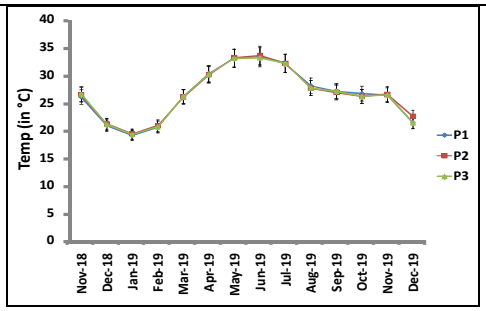

Fig 3. Temp. (⁰C) in three ponds (Average value) (Nov, 2018-Dec, 2019)

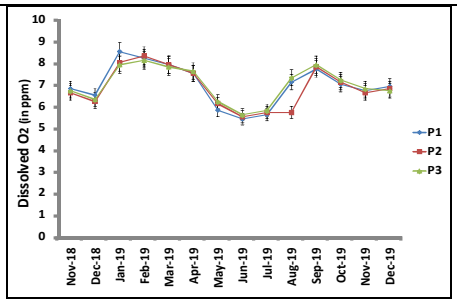

Fig 4. Dissolved oxygen (DO) in three ponds (in ppm) (Nov 2018-Dec-2019)

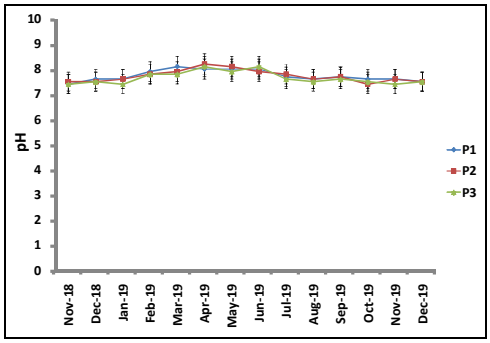

Fig 5. pH in three ponds (Average value) (Nov 2018-Dec-2019)

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REVIEW ARTICLE

Rainfall Prediction using Computational Intelligence Techniques: A Review

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ABSTRACT

Rainfall Prediction is considered to be one among the challenging phases in Forecasting Weather. There are many merits of accurate and timely prediction of rainfall. It helps in taking preventive measure against agricultural difficulties, flood situations etc. The fields like agriculture, aquatic life, and ecosystem get affected of it. To get the real rainfall information, various statistical methods are proposed in the literature. Due to dynamic nature of atmosphere, statistical techniques fail to provide good accuracy for rainfall forecasting.Nonlinearity of rainfall data makes Artificial Neural Network a better technique. Review work and comparison of different approaches and algorithms used by researchers for rainfall prediction are analysed in this paper. The main aim of this paper is to give non-experts an easy access to the computational intelligence techniques and approaches used in the field of rainfall prediction.

Keywords: Rainfall Prediction, Neural Network, Computational Intelligence Model, Expert System,MLP

INTRODUCTION

Rainfall is a natural phenomenon. Rainfall Prediction is regarded as a challenging task in meteorology. It has prime importance in the areas like science and research, marine biology etc. Rainfall Prediction is difficult to perform as well as a challenging task. One of the prime reasons for it is the dynamic changes in climate and atmospheric process. Therefore accuracy in Predicting Rainfall is the major challenge for Meteorology Department [1]. Accurate Prediction of rainfall is not possible as it cannot be predicted where the rainfall will occur and whether it is a heavy

rainfall or not. The common factors, which affect the occurrence of rainfall, are temperature, humidity, wind speed, motion of cloud etc. It helps in saving life and assets and does disaster management caused due to heavy rainfall. Therefore to impart an accurate prediction, a set of prediction models have been devised and implemented. This Paper has the objectivity of going through various models relating to computational intelligence. Many Researchers have applied a set of techniques for rainfall prediction and tried developing certain technologically advanced monitoring System by implementing and integrating Artificial Neural Network, Genetic Algorithm [2].MLP also helps in predictions, Genetic Algorithm is applied for inputs, structure between the inputs, the output layers and to make the training of Neural Network more effective [3].

LITERATURE STUDY OF RAINFALL PREDICTION METHODS

Rainfall Prediction plays an important role in the horticulture, agriculture, water resource management, crop production plan. This prediction has a vital role in serving to the mankind. The researchers predict rainfall with accuracy with the help of different number of approaches. Few methods are accurate than the others [4]. Weather Prediction is a method, which gets data basing on atmospheric conditions. It records the different atmosphere parameters like humidity, temperature, wind speed, rainfall, direction and so on. Different number of tools can be used for getting the data for forecasting the weather. Those tools may be wireless sensors, radars, high speed computer systems, meteorological satellites etc [5]. Weather forecast has a number of advantages, like monitoring and observing climate or weather, overcoming climate hazards, agriculture production, detection of drought , aviation industry and so on. In general, a large amount of weather data are available with different sources like meteorology department website, UCI , Kaggle Repositories etc. These are considered as rich information and utilised for prediction. Different Data Mining Techniques are used with available weather data for predicting atmospheric parameters. These parameters cited above are dynamic in nature [6]. Weather calculation with atmosphere parameters change with the geographical location. The Data Mining Techniques, used for weather prediction include Fuzzy Logic, Artificial Neural Network (ANN), Regression, Decision Trees, Naive Bayes, and Support Vector Machines (SVM) etc.

Fuzzy Logic

Fuzzy logic is known as Fuzzy Inference System (FIS).Fuzzy logic has two components, Knowledge base and database. Knowledge base is composed of a set of if then rules whereas database defines the membership function. Fuzzy Logic relies on recognition. Here logical statements are taken, but not restricted with true or false values. It ranges with “almost certain” value to “very unlikely” [7]. Fuzzy logic plays a vital role in expert system applications.

Fuzzy inference system (FIS) has following blocks,

1. Rule base-It consists of if-then rules
2. Membership functions- It uses fuzzy rules
3. Decision making Unit- It performs inference operations
4. Fuzzification Interface- It converts the crisp inputs to degrees of match with linguistic values
5. Defuzzification Iinterface- It transforms the fuzzy inference results to crisp output.

Following Figure implies the structural representation of Fuzzy Inference System.

ANN (Artificial Neural Network)

Artificial Neural Network (ANN) is an information processing structure. It is inferred from the biological nervous system. Biological Nervous System consists of brain and processing information [8]. It is consisting of interconnected processing elements known as neuron. Its objective is to solve some specific problem.ANN is a flexible arithmetic structural representation. It finds critical nonlinear relationship between input and output data set. Artificial Neuron Network Models are necessary. They are also efficient. The Processing elements are connected by synoptic weights. They adapt through a learning process [9]. In this era, Artificial Neural Networks have been found with application in vision, pattern recognition, classification, speech recognition, and control systems.

Regression

A statistical approach, which tries to get the conclusion of the strength of the relationship between one dependent variable and a series of other independent variables is known as Regression [10]. A Regression Model contains two and more number of predictor variables. These are known as Multiple Regression Model [11].
Dependent variable is taken as Y and independent variable as X.
Multiple regression model is of the following form:

$$Y=a0+a1x1 +a2x2 +a3x3+ a4x4+... .e$$

Where a0, a1, a2, a3, a4 are known as the regression coefficient, e is the unexplained portion of dependent variable with zero mean along with constant variance [12].
Multiple regression is used as a model to predict a dependent variable from two or more independent variables [12] .

Naive Bayes

Naive Bayes classifier is a simple approach of Bayesian network. Naive Bayes class has no parents. Single attribute is having parent, which is class. The model is built without counting complex parameters [13].For large data sets, the classification method is applicable. The approach has explicit model for deployment. It can be applicable for any real world issue. Minimal training data can be used for prediction of classification parameters [14]. The methodology is usually applied to predict rain fall.

Multilayer Perceptron (MLP)

MLP, which stands for Multi Layer Perceptron is called Feed Forward Network. It belongs to Artificial Neural Network (ANN). It is composed of non linear activation function. This function is present in hidden layer. Input and Output vectors perform nonlinear mapping [15]. There are two functions,
1. Pattern Classifiers
2. Nonlinear Adaptive Filters
The neural network consists of three layer architectures, 1. Input layer defines input value, 2.hidden layers defines the mathematical function, 3. Output layer defines final outcome of each layer. The set of neurons are interconnected with weights [16]. Neuron has activation function. It takes input with the earlier layer, yields output for the later one. The Activation Function counts the number of Predictions [17].

Support Vector Machines (SVM)

Support Vector Machine is a multi layer feed forward network. Support Vector Machines can be used for pattern classification and nonlinear regression. Support Vector Machines was developed by Vapnik and his co-workers. Its application is for supervised learning[17]. The reason for it is better generalization performance compared to Neural Network model. SVM result is unique, optimal. SVM is a method, which solves a number of classification problem, Kernel PCA, Kernel based clustering, feature selection, and dimensionality reduction. Some researchers have used the technique to predict rainfall to find accurate output. Support Vector Machines (SVM) with linear or nonlinear kernels is a learning algorithm used for the classification and regression. These are the methods in data mining with kernel mapping. SVM is a set of supervised learning methods. SVM is an extension to nonlinear models of the algorithm [18].

Decision Tree

One of the predictive modelling approaches is Decision Tree. It can be used in prediction, classification, and clustering. It uses a technique, Divide and Conquer, which decomposes the problem into number of subsets [19]. The Decision Trees consists of two parts,
1. The growth of the tree to enable it to accurately categorize the training dataset
2. The pruning stage is a methodology in machine learning as well as searching algorithm to decrease the size of decision tree. It overcomes the classifier issues thereby increasing the predictive accuracy.

CONCLUSION

This paper is intended to provide an analysis of a no. of rainfall prediction methodologies used by different researchers. It helps generating a prediction model in getting rainfall accuracy by implementing any of the techniques cited.

REFERENCES

1. Shivam Bang, Rajat Bishnoi, Ankit Singh Chauhan, Akshay Kumar Dixit, Indu Chawla."Fuzzy Logic based Crop Yield Prediction using Temperature and Rainfall parameters predicted through ARMA, SARIMA, and ARMAX models",2019 Twelfth International Conference on Contemporary Computing (IC3), 2019
2. Jesleena Rodrigues, Arti Deshpande "Prediction of Rainfall for all the States of India Using Auto-Regressive Integrated Moving Average Model and Multiple Linear Regression",2017 International Conference on Computing,Communication, Control and Automation (ICCUBEA), 2017
3. Chandrasegar Thirumalai, Swapna Anupriya Chandhini, M Vaishnavi. "Analysing the17concrete compressive strength using Pearson and Spearman", 2017 International conference of Electronics, Communication and Aerospace Technology (ICECA), 2017
4. Zaini, Nuratiah, Marlinda Abdul Malek, and Marina Yusoff. "Application of computational intelligence methods in modelling river flow prediction: A review", 2015 International Conference on Computer Communications and Control Technology (I4CT), 2015.
5. J. Rodrigues and A. Deshpande, "Prediction of Rainfall for all the States of India Using Auto-Regressive Integrated Moving Average Model and Multiple Linear Regression," *2017 International Conference on Computing, Communication, Control and Automation (ICCUBEA),* Pune, 2017, pp. 1-4.
6. Chandrasegar Thirumalai, K Sri Harsha, M Lakshmi Deepak, K Chaitanya Krishna "Heuristic prediction of rainfall using machine learning techniques", 2017 International Conference on Trends in Electronics and Informatics (ICEI), 2017
7. Pinky Dutta, Saikia, Hitesh Tahbilder, "Prediction of rainfall using data mining technique over Assam", IJCSE, vol. 5, no. 2, pp. 85-90, 2014.
8. Dubey and D. Akash, "Artificial neural network models for rainfall prediction in Pondicherry", International Journal of Computer Applications, Vol. 120, No. 3, 2015.
9. Ahmed, Bilal, "Predictive capacity of meteorological data: Will it rain tomorrow?", Science and Information Conference (SAI), 2015, IEEE, 2015.
10. B. Kavitha Rani, A. Govardhan, "Rainfall Prediction Using Data Mining Techniques - A Survey", ITCSE ICDIP ICAIT, 2013.
11. AllaManasa, M. Rajinikanth, Rainfall Forecasting Using Data Mining Technique.
12. AchmadAndani, Statistic Approach versus Artificial Intelligence for Rainfall Prediction Based on Data Series, 2013
13. M. Kannan, S. Prabhakaran and P. Ramachandran, "Rainfall forecasting using data mining technique", 2010
14. S. Asadi, J. Shahrab, P. Abbaszadeh and S. Tabanmehr, "A New Hybrid Artificial Neural Networks for Rainfall-Runoff Process Modeling." Neuro computing.Vol 121 (2013): 470-480.
15. A. M. Kalteh, "Rainfall-Runoff Modelling Using Artificial Neural Networks (ANNs): Modelling and Understanding," Caspian J. Env. Sci, 2008, Vol 6 (1): 53-58.
16. V. Nourani and M. Komasi, "A Geomorphology-Based ANFIS Model for Multi-station Modeling of Rainfall-Runoff Process," J. Hydrology, Vol 490 (2013): 41-55.
17. Pritpal Singh, Bhogeswar Borah, Indian summer monsoon rainfall prediction using artificial neural network, springer 2013

18. K. H. Wang and A. Altunkaynak "Comparative Case Study of Rainfall-Runoff Modeling between SWMM and Fuzzy Logic Approach." *J. Hydrologic Engineering*, 2012, Vol 17 (2): 283-291.
19. R. R. Deshpande, "On the rainfall time series prediction using Multilayer Perceptron Artificial Neural Network," Int. J. of Emerging Technology and Advanced Eng., vol. 2, no. 1, pp. 148-153, 2012.

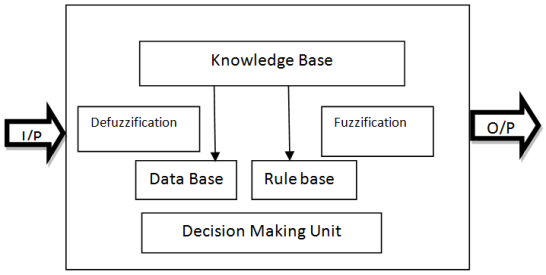

Fig 1-General Structure of FIS

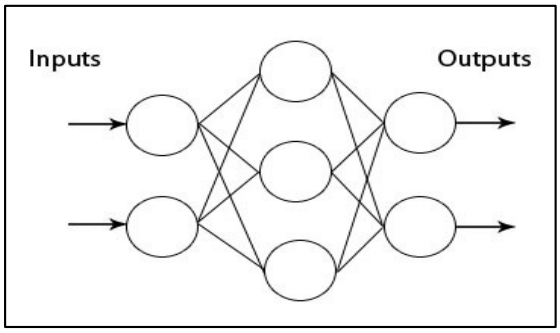

Fig 2- ANN

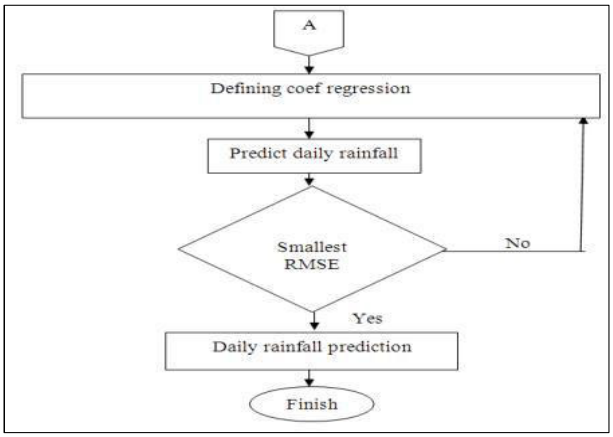

Fig 3: Regression steps

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REVIEW ARTICLE

A Review on Human Facial Recognition Techniques

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ABSTRACT

Face of a human being is an important part. One person can be differentiated from the other with the help of it due to some unique features associated. Biometrics is one of the important area, where Facial Recognition plays a major part. Scope of this paper is to review on facial recognition. It has the objectivity to find and survey different Facial Recognition Techniques. These are the real world applicabilities in the area of Artificial Intelligence and Machine Learning. This acts as a frame work for real time face recognition and recognition. Face recognition is regarded as a technology which considers the position and dimension of a face in digital image. This Paper is intended for presenting a comprehensive review of Facial Recognition Techniques.

Keywords: Facial Recognition, Artificial Intelligence, Machine Learning Methods

INTRODUCTION

Biometric techniques are identification based. The Parameters are the physiological characteristics like face, fingerprints, finger geometry, hand geometry, hand veins, palm, iris, retina, ear, voice etc. Face Recognition has advantages over the Biometric methods. Face Recognition is beneficial for security and surveillance purpose. Face Recognition is a visual pattern recognition problem. Face is a three-dimensional object, which vary with illumination, pose, expression and so on. Face identification can be viewed as a particular instance of article class recognition. In object class identification, the errand is to discover the areas and sizes of all articles in a picture that have a place with a given class. Models incorporate upper middles, people on foot, and cars. Face-location calculations center on the recognition of frontal human countenances [1]. Users are capable of identifying the faces by learning throughout life

span, recognize the familiar faces after distance of years. The human beings are capable of it irrespective of being affected after the lapse of the period and some visual changes. These changes are occured due to issue in aging, distractions, different facial conditions like growing beards on face, hair style changes, wearing of glasses, expressions etc. The face detection has the objective to find whether face in any image exists or not. It is an important task for human beings, which is a challenging task for computer systems [2]. Now a days, it has been considered one important research topics.

Facial Recognition Techniques

A number of technologies are used for face identification from the images. Facial Recognition System identifies faces present in the images and videos. It is divided into following categories:

1.Facet authentication, which is also used for authentication: one to one matching is done here. It compares a query face image against a pattern of features image which checks for the identity.

2. Face Identification : here a number of and kind of compare are being done. it contrasts a query face image aligned with the face patterns available in the database to decide the distinctiveness of the reserved face image.[3][4]

When any Algorithms on Facial Recognition are to be developed, then system test is being made. For Face Identification Classification testing, a collection of faces are required. A standard database is always used. There are plentiful standard collection being offered and any proper database can be certainly chosen as per requirement [4]. Some popular databases include FERET database, AT&T Face Database, UCI Repository, AR Database, Yale Database, Kaggle etc.

Template based Method: Template matching is a concept, which is related to an approach to spot the faces with help of global representations. These methods include certain processe. face image is taken as a whole and extracts features from the whole face region and then classify the image by applying a pattern classifier. One of the methods used to extract features in a holistic system and it is based on statistical approaches [5].

Statistical Methods: There methodologies identify, analyse and parameterize the linear subspaces. There are some statistical face recognition techniques excluding the linear subspaces. These are based on nonlinear subspaces. Non linear subspaces include kernel-PCA and kernel-LDA, Transformation (Hidden Markov Model (HMM), Fourier Transform) and Support Vector Machine (SVM)[6].

Neural Network: Neural Network or Artificial Neural Network (ANN) is a popular tool for pattern recognition problems. One of the demonstrations of neural network for face image has applications. Using a small set of face images, accurate recall was reported even when input image is very noisy, low resolution and dimension or when portions of the images are missing [7]. ANN consists of simple elements, operated in parallel.ANN can be used for Facial Classification and Gender Classification. ANN are used to reduce the complexity. The neural network learns from experience, works on the images with change in lighting conditions and improves the accuracy. The major drawback of the neural network is large amount of time required for training.ANN finds the face with help of learning. NN based system is trained, so that it can be able to recognize the faces. Neural Network with Incremental Learning Ability was used for the face recognition purpose [7][8].

Hidden Markov Model (HMM): It is a statistical model. This HMM has two processes. One is Markov Chain with a finite number of states [9].This can't be viewed. The second process consists of states. Each state has a set of probability density function associated with it. This model is analogous to Eigenface method. The Hidden Markov Model has a great contribution in the area of speech recognition. But This Model had the objective to identify the faces.HMM is applicable for facial recognition, face detection, object recognition etc. The number of states can be increased or decreased depending upon the system's requirement. HMM also raises the performance of the face recognition system [10].

Support Vector Machine (SVM): SVM is a method dealt with the classification issues. SVM is a machine learning method, where the classifier is trained sufficiently and effectively, which deals with the face recognition issue. SVM takes out the discriminatory information from the training data. SVM works to find the classification. The scope with SVM is dealing with the two class predicament. Face Recognition is a Multi class problem [10][11]. Use of SVM does the face recognition after facial feature extraction is made. For face recognition, SVM can be applied individually or can be used with the other techniques. Like a Hybrid method can be used in which features can be extracted with Independent Component Analysis (ICA) and then afterward the recognition issue can be resolved using SVM[13][14].

Facial recognition is regarded to be one of the active areas of research since many years. The Face Recognition consists of several areas like machine learning, image processing, computer vision, pattern recognition, neural networks. It mainly helps in security systems, surveillances, biometrics, law Enforcement etc [5]. Here the main constraint is Classification. Facial Recognition methods include training of facial images from the given set of data, classify the new test images into one of the classes. The problem of Face Recognition can be resolved by humans. The machine learning face recognition system has some disadvantages. They are ageing, facial expressions, scaling factors, illumination variance etc [6][12].

Luo et al. (2018) have suggested deep cascaded detection method that iteratively exploits bounding box regression, a localization technique, to approach the detection of potential faces in images. They also consider the inherent correlation of classification and bounding-box regression and exploit it to further increase overall performance. Their method leverages cascaded architecture with three stages of carefully designed deep convolutional networks to predict the existence of faces [16]. Tensor Flow is a machine learning system that operates on large scale and in heterogeneous environments. Tensor Flow uses dataflow graphs to represent computation, shared state, and the operations that mutate that state. It maps the nodes of a dataflow graph across many machines in a cluster, and within a machine across multiple computing devices, including multi core CPUs, general purpose GPUs, and custom-designed ASICs known as Tensor Processing Units (TPUs).

Stitiprajna et al.(2020) have used the Haar-Cascade classifiers for the extraction of features. They have downloaded the xml file of Haar-Cascade from Google and saved in directory. A no. of features have been found to be encoded within it. By the help of this classifier they have detected the faces. They have taken a 3×3 dimension matrix and passed it across one image taken. At each move, the pixel at the centre is compared with pixels all across. Hence they have found out a threshold value. The neighbours are denoted by intensity value, which is less than or equal to the centre pixel by 1 and the rest by 0.After reading these 0 or 1 value in the 3×3 dimension matrix, a binary pattern like 11100011 is found, which is local to particular area of the image. By applying on the image, a set of local binary patterns will be get. After training the images, the authors have used LBPH algorithm and with the help of the histogram, are able to recognize the faces of the given data. The proper path have been given to the folders where the images of the persons exist. After it, the video streaming have been made through the web camera. It will detect the photos in the video frame by frame and show the name of the person. Current time and date modules have been imported for showing in which time and date that it had recognized the faces.Mukherjee et al. (2017) have discussed the methods, using hand crafted features followed by training a simple classifier and an entirely modern approach of learning features from data using neural networks. Ren et al. (2017) have presented a method for real time detection and tracking of the human face. The proposed method combines the Convolution Neural Network (CNN) detection and the Kalman filter tracking. Convolution Neural Network (CNN) is used to detect the face in the video, which is more accurate than the traditional detection method. Kalman Filter [16] is used, when the face is largely deflected or severely occluded. Tracking is utilized to predict the face position. They try to increase the face detection rate, while meeting the real time requirements.

CONCLUSION

This Paper discusses about the recent development in the field of face recognition and the methodologies adopted to achieve. Facial Recognition Systems have reached certain height while operating under constrained conditions. The lists of references have the objective to understand the process easily. The Face Recognition in video has more challenges to the current face recognition systems.

REFERENCES

1. Stitiprajna Panda, Swati Sucharita Barik, Sasmita Kumari Nayak, Aeisuriya Tripathy, Goura Mohapatra,Human Face Recognition using LBPH, https://www.ijrte.org/download/volume-8-issue-6/
2. Sennaar, K. Facial recognition applications – security, retail, and beyond,https://emerj.com/ai-sector-overviews/facial-recognition-applications/ (accessed 14 June 2019).
3. Kaur, P, Krishan, K, Sharma, SK, et al. Integrating a profile of frontal face with its mirror image for facial reconstruction. J Craniofac Surg 2018; 29: 1026–1030.
4. Luo D, Wen G, Li D, Hu Y, Huan E (2018) Deep-learning-based face detection using iterative bounding-box regression. Multimed Tools Appl. https://doi.org/10.1007/s11042-018-5658-5
5. Mukherjee S, Saha S, Lahiri S, Das A, Bhunia AK, Konwer A, Chakraborty A (2017) Convolutional neural network based Face detection. In: Proceeding of 1st international conference on electronics, materials engineering and nano-technology, pp 1–5
6. Ren Z, Yang S, Zou F, Yang F, Luan C, Li K (2017) A face tracking framework based on convolutional neural networks and Kalman filter. In: Proceeding of 8th IEEE international conference on software engineering and service science, pp 410–413
7. Fontaine, X, Achanta, R, Süsstrunk, S. Face recognition in real-world images. In: IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), New Orleans, LA, 5–9 March 2017, pp.1482–1486. Piscataway, NJ: IEEE.
8. Singh, M, Arora, AS. Varying illumination and pose conditions in face recognition. Procedia Comput Sci 2016; 85: 691–695.
9. Agrawal, AK, Singh, YN. Evaluation of face recognition methods in unconstrained environments. Procedia Comput Sci 2015; 48: 644–651.
10. Asavari G. Joshi and A. S. Deshpande, "Review of Face Recognition Techniques", International Journal of Advanced Research in Computer Science and Software Engineering, vol. 5, Issue no. 1, 2015.
11. Marryam Murtaza, Muhammad Sharif, Mudassar Raza, Jamal Hussain Shah, "Analysis of Face Recognition under Varying Facial Expression: A Survey", The International Arab Journal of Information Technology (IAJIT) Volume 10, No.4 , July 2013
12. Murtaza, Marryam, et al. "Analysis of Face Recognition under Varying Facial Expression: A Survey." *International Arab Journalof Information Technology (IAJIT)* 10.4 (2013).
13. Ambika Ramchandra and Ravindra Kumar,"Overview Of Face Recognition System Challenges," International Journal of Scientific & Technology Research (IJSTR), vol. 2, issue 8, Aug.2013.
14. Muhammad Sharif, Muhammad YounasJaved, SajjadMohsin,"Face Recognition Based on Facial Features", Research Journal of Applied Sciences, Engineering and Technology 4(17): 2879-2886, 2012
15. Thorat, SB, Head, SKN, Jyoti, M, et al. Facial recognition technology: an analysis with scope in India. Int J Comput Sci Inf Secur 2010; 8: 325–330.
16. Shou-Jen Lin, Chao-Yang Lee, Mei-hsuan Chao, Chi-Sen Chiou, Chu-Sing Yang, "The Study And Implementation Of Real-Time Face Recognition And Tracking System", Proceedings of the Ninth International Conference on Machine Learning and Cybernetics, Qingdao, 11-14 July 2010.

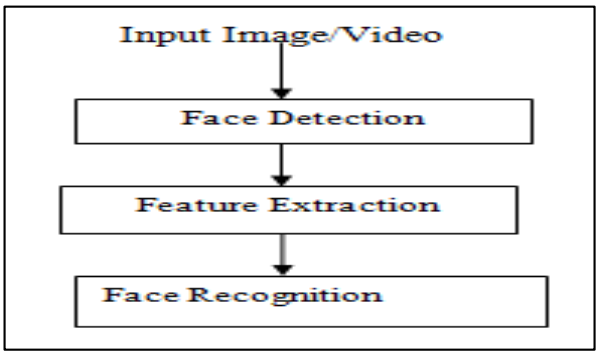

Fig 1: Facial Recognition System

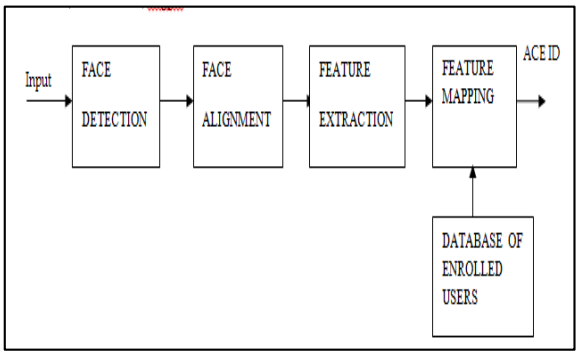

Fig.2: Face Recognition Process Flow

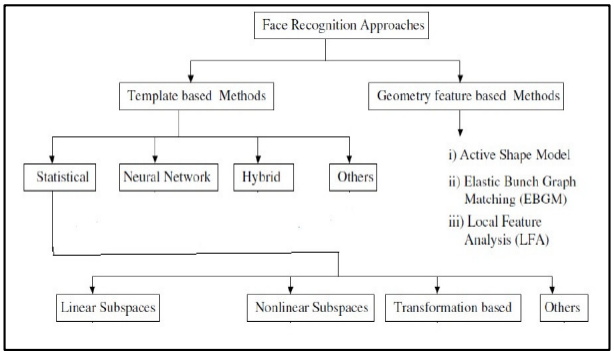

Fig 3: Facial Recognition Approaches

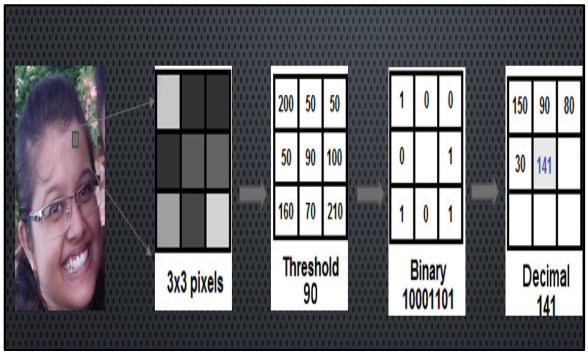

Fig.4: Image Thresholding [1])

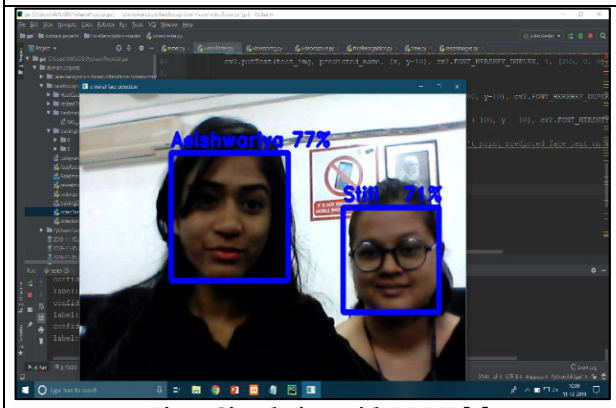

Fig.5: Simulation with LBPH [1]

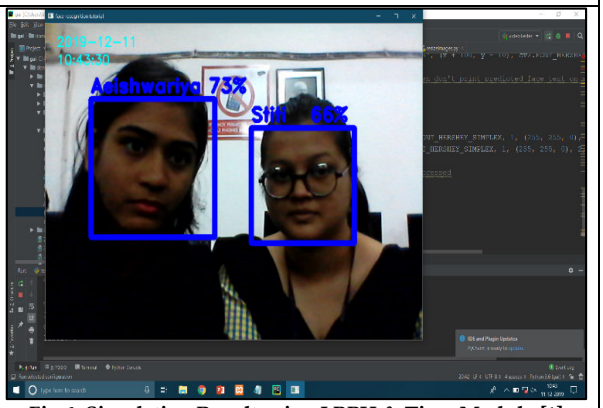

Fig.6: Simulation Result using LBPH & Time Module [1]

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RESEARCH ARTICLE

Effect of Dietary Calcium Level on Egg Shell Quality of Aged Laying Hens Housed In Conventional Cage

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ABSTRACT

This experiment was guided to investigate the effect of dietary calcium level on eggshell thickness of aged laying hens. With increasing hens age increased the egg size and weight, but it not directly proportional to the shell weight, which gives on to decreased in the shell thickness as well as the shell weight in egg weight ratio. The eggs are cracked due to weak eggshell. More numbers of cracked eggs are view in aged layers could be result of disturbance with the calcium homeostasis. Due to calcium deficiency calcium were supplying needed to make a good shell. So, in this experiment total 24 numbers of hens, 45to 50 weeks old Vanaraja hens were used and housed in conventional cages and divided into 4 groups and each group fed with diet containing calcium level of 3.8%, 4.1%, 4.5% for 10 weeks and another one group is under control. The feed diet containing corn, wheat, soybean meal, oat, calcium and vitamin D3 tablet. After 4- 10 weeks of feeding, the eggs from each group were collected individually and the external parameters of these eggs were measured. This experiment had no effect on the eggshell qualities' traits such as eggshell thickness, eggshell weight. Thus, this experiment suggested that the aged reproducing hens requires sufficient level of calcium every day in their diet.

Keywords: Dietary Calcium Levels, Cracked Eggs, Eggshell quality, Aged laying hens, eggshell thickness.

INTRODUCTION

Technically poultry is termed for those species of birds that has been domesticated to produced and grow in captive condition for their meat and egg. In India the word poultry is synonymous with domestic chicken (*Gallus gallusdomesticus)* because other type of poultry almost unknown as source of egg and meat (Alemu, 1995).

Egg

According to the intake of food, egg is considered aslow cost but it contains highly nutritious substances, which provides balanced nutrients and have a great impact on human health. Eggs contain essential protein, selenium, fats soluble vitamins, minerals, and bioactive compounds. Composition and net amount of egg depends on age, hen foodstuffs, and environmental situations. The ratio of nutrient to energy density of one egg (50g) contains 78 kcal is energy,6.29gis saturated,2.0g is monounsaturated, 0.7g is polyunsaturated, and 186mg is cholesterol. Egg also contains micronutrients but doesn't contains vitamin C and also contains variety of minerals like eggshell contains high amount of calcium also the yolk contains small amount of calcium, iron, magnesium, phosphorous, potassium, sodium, and zinc) all of these are important ingredient in egg and most vitamins are present in egg.

Egg Proteins

Egg is highly proteinaceous and it is an important ingredient in human diet. It proved to be having antioxidant like phosvitin, which is present in egg white. The evaluation of external and internal quality of egg is essential as consumer prefer to better quality of eggs (Song et al., 2000). According to (Stadelman1997) egg is compost of those quality characteristics which affect its acceptability to consumers such as cleanliness, freshness, egg weight, shell quality, yolk index, albumin index, Haughunit and chemical composition. According to(Swiatkiewicz et al., 2015) eggshell quality is one of the significant issues in the egg industry. The calcium enters the shell structure up to 95% as calcium carbonate and represents 1.5% of body weight of the hens so that calcium is the most important nutritional factor determining eggshell quality (Gerber, 2006, Swiatkiewicz et al., 2015). Another scientist (Robert, 2004) told thateggs with inferior shell quality are a leading economic loss to poultry producers. According to (Roland 1988)it has been reported that the average of eggs cracked and lost prior to point of consumption ranged from 13% to 20%. Due toreduce in an intestinal Ca uptake, which causes decrease in eggshell thickness and increased egg sizein aged laying hens (Al-Batshan et al., 1994). Increases in hens age, egg size and egg weight increased, but it is not directly proportional to the shell weight, which conduct to decrease in the shell weight in comparison with egg weight ratio.So,a greaternumberof cracked eggs are found mainly in late old age period of hens.

(Elaroussi et al., 1994) suggested that the increase in ruptured eggs view in old age laying hens could be a result of disruption related with the calcium homeostasis. According to (Ahmed et al., 2013)calcium is the one of the solutionswhich is required for egg production and optimal egg shell quality of laying hens. (Roland (1987) also suggested that anincreased in egg shell quality when feeding dietary Ca above 4.35 g/d. On the other hand, (Leeson et al., 1993) did not find any difference on the eggshell quality when the laying hens fed with high level of dietary calcium and come to the conclusion that 3.4 g Ca per daywassufficient for brown egg layers. The domestic chicken that is *Gallus gallusdomesticus* (2n=78) is comes under Family Phasianidae and Order Galliformes.

Calcium

Calcium is the most important nutrientin the formation and metabolism of bone. Both calcium and phosphorus are needed for the formation of bone. It also provides mechanical strength. Freshly hatched chicks require an immediatesupply of calcium in their diet for bone development.

METHODS AND METHODOLOGY

The study was carried out in Centurion University of Technology and Management, Bhubaneswar. In this experiment 24 number of hens, 40-50 weeks old Vanaraja hens were used and housed in conventional cages. Then the layers were divided into 4 groups, one group contains 6 numbers of birds under control and other 3 groups are feed with dietary Ca level and each group contains 6 numbers of birds. The layers were provided with one of the experimental diets with calcium level 3.8%, 4.0%, 4.5% respectively. And the control was also taken with numbers of hens with same age. All diets were getting ready to meet and exceed the nutrient demand of (NRC, 1994). Ingredient

compositions of diets were corn, wheat, soybean meal, oats and calcium and vitamin D_3 tablets. The experimental was conducted for 10 weeks, at that time room temperature was 25to 5 C.Feeds were freshly added daily.
Moisture of nutrient was measured by using the oven, before kept the nutrient in the oven measure the weight and then kept it into the oven overnight at 100 C. Crude fat measured by the help of succilator and rotary evaporator. Crude protein was measured by Lowry method.

Egg Production and Qualities

The egg produced by the experimental hens was recorded and measuring the average weight of egg and also excluding the abnormal eggs. The percentage of cracked eggs were calculated per each group (number of broken egg / numbers of egg produced × 100). At 6, 8 and 10 weeks of experiments,6eggs from each group were collected and measuring the egg individually.Then measuring the internal and external qualities of eggs.

External Egg Quality Parameters

1. Egg weight was measured bythe help of weighing machine (Aczet _ model_CY224).
2. Egg width and egg length were measured with aVernier calliper in centimetres.
3. shape index of the egg was obtained by the shape indexformula, for primarily measuring the egg quality.
   Shape index = width of the egg ÷length of the egg×100.

Internal Egg Quality Parameters

The internal egg quality of individual egg sample was measured by breaking them on a uniform white surface and being careful not to breaking the vitelline membrane that enclosed the yolk. The parameters were measured as follows.

1. Yolk width was measured as the widest horizontal circumference with Vernier calliper in centimetres.
2. Yolk height was measured as the height of yolk at the midpoint with tripod micrometre

Yolk index= height of yolk÷ width of yolk

1. Albumin height of the eggs were broken and albumin height were measured from at least three places with tripod micrometre.
2. Albumin width was measured as the widest horizontal circumference of the thick albumin with a Vernier calliper in centimetre.

Albumin index = height of albumin ÷width of albumin

1. Shell thickness of dry egg shell was measured with micrometre screw gauge. The mean point (the narrow, the broad and middle) were taken as the shell thickness.
2. Haugh unit basically measure egg protein quality, on the basis of egg albumin. For measuring Haugh unit the egg was broken on a white flat surface plate, during these always avoiding the breakage of yolk and by using tripoid micrometre the height of thick albumin was measured. Haugh unit was resolved by using the formula as follows

$HU= 100\log (H+7.57-1.7W^{0.37})$
Where HU= Haughunit
H= height of albumin(mm)
W= weight of egg
The experimental data was obtained by statistical analysis with the help of analysis of variance (ANOVA) and the significant difference between the mean were calculated.

RESULT AND DISCUSSION

The feed intake of oldagelaying hens with varying ca levels were represented in Table 1 and the analysed composition of the diet were represented in table 2. The diet containsCa levels didn't affect feed intake, egg production and egg weight significantly. In increasing ca level 4.0g to 4.5g in diet cracked egg reduced linearly ($p< 0.01$). A number of studies have been resulted that laying performance was not significantly affected by the dietary calcium level in laying hens. (Cufardaret al.,2011) in their experiment when the laying hens feeding with 3.0%, 3.6%, 4.2% of Ca in their diet, the scientist didn't find any significant effect on egg production and egg weight. Frost and Roland (1991) and keshavaraz and Nakajima (1993) also suggested that different level of dietary Camake an effort a negative effect on egg production as aresult of reduce feed intake (Ousterhout, 1980; Pelicia et al., 2009).

In this experiment the feed intake varies from 100.2- 102.4 g. There was no negative effect on egg production. There have been finding a conflicting relationship among feed intake after feeding diets with varying level of calcium. (Olver and Malan 2000) point out that the dietary calcium levels did not impact total feed consume during 16 to 80wks of age. (Narvaez- Solarteet al.2006) reported that daily feed consume was decreased as Ca levels in the diet increased. While (Chandramoni et al., 1998) reported that with increasing the level ofCain the diet, the daily feed consumption tended to be increase, but not significantly. This lack of consistency may be due to the difference in hens age, feeding level of Ca, dietary energy density. Significantly reduced in incidence of cracked egg with increasing Ca level, which was might be related with improvement in eggshell thicknessseen in (Table 4) asincreasing dietary Ca. when the laying hen'sintake of insufficient amounts of Ca in their diet may causes poor shell quality which leads to higher occurrence of cracked eggs (Jiang et al., 2013). In this experiment feed intake was not affected by dietary calcium level, but the calcium intake increases as dietary calcium increases. To decrease the incidence of cracked eggs in old age layers, the diet must contain enough Ca due to the effect being liner.

Eggshell Qualities

Egg and eggshell qualities of old agelaying hens fed diets with varying level of Ca are represented in Tabel 4. As Ca level increases in the dietHaugh unit score was linearly increased. The egg shell quality was influenced by Ca levels in the diet.

Egg shell thickness measurement is expressed as 0.01mm.
Dry egg shell weight was measured by weighing machine (Aczet_model_CY224).
Haugh unit value is determined using the procedure describe by Haugh (1937).
$HU= 100\times\log (H+7.57-1.7\times W^{0.37})$
The effect of Ca levels on egg shell qualities are incompatible with the available result. According to (Jiang et al., 2013) layers fed on a diet with 2.62% Ca had a weaker eggshell breaking strength as compare with those old laying hens fed with diet contain 3.7% or 4.4% level Ca. Another scientist (Roland 1987) suggested that the eggshell thickness was linearly increased when diet containCa levels were above 4.35g per day. On the other hand (Cufadar et al., 2011) also noted that the level of Ca on the diet had no significant effect on incidence cracked eggs and eggshell thickness. On the other hands, (Keshavarz and Nakajima, 1993) suggested that increasing levels of Ca from 3.5% to 5.5 % in the diet did not have any beneficial effect on eggshell qualities in a long-process experiment. The adequacy amount of Ca for optimal eggshell qualities is stillunder experiment. But this experiment was conducted based on the result and suggestion from the previous studies, a constant increase in the dietary Cahas been associated with the increase in the eggshell qualities. (Castillo et al., 2004) concluded that 4.26% of calcium in the diet is the biological optimum level for maximum eggshell quality. An increase in Cainthediet from 4.08 to 4.64 g/d which reduce incidence of cracked eggs and improve the eggshell weight and egg shell thickness in aged Brown layers (Safaa et al., 2008), which is similar with this study.

(Pelicia 2009) suggested that taking 90 and 108 weeks of old age laying hens in the experiment, there was no effects of Ca on eggshell quality; but the eggshell percentage and eggshell weight per surface area (ESWSA) was increased by increasing Ca concentration in the diet. The (NRC 1994) reported the Caneededfor Brown layers to be 3.4% of dietary Ca for 110g/d feed consumenevertheless of age, which seems insufficient for optimal eggshell qualities.

REFERANCES

1. Ahmed, N. M., K. A. Abdel Atti, K. M. Elamin, K. Y. Dafalla, H. E. Malik, and B. M. Dousa. 2013. Effect of dietary calcium sources on laying hen's performance and egg quality. J. Anim. Prod. Adv. 3:226-231.
2. A1-Batashan, H. A., S. E. Sceideler, B.L. Black, J. D. Garlich, and K. E. Anderson. 1994. Duodenal calcium uptake, femur ash and eggshell quality decline with age and increase following moit. Poult. Sci. 73:1590-1596.
3. Alemu Y 1995 Poultry production in Ethiopia. Worlds Poultry science Journal, 51, 197-201.
4. AOAC (Association of Official Analytical Chemist) Intenational. 1995. Official Method of Analysis of AOACInternational,16thedn. AOAC International, Gaithersburg, MD, USA.
5. Balnave, D.,El-Khatib, N.U. AND Zhng, D.(1992). Calcium and carbonate suppy in the shell gland of hens laying egg with strong and weak shells and after arrest from lay.Poult.sci.71;2035-2040.
6. Bar, A. & Hurwitz, S. (1987). Vitamin D metabolism and calbindin (Calcium- binding protein) in aged laying hens. The Journal of nutrition,117(10):1775-1779.
7. Bar, A., Razaphkovsky, V.&Vax, E. (2000). Re- evolution of calcium and phosphorus requirement in aged laying hens. British poultry science, 43 (2):261-269.
8. Bar,A,(2009). Calcium transport in strongly calcifying laying birds: mechanism and regulation. Comparative Biochemistry and Physiology part A: A Molecular & Integrative Physiology, 152 (4),447-469.
9. Blokhuis, H. J., T. Fiks van Niekerk, W. Bessei, A. Elson, D. Guèmenè, J. B. Kjaer, G. A. Maria Levrino, C. J. Nicol, R.Tauson, C. A. Weeks, and H.A. van de Weerd. 2007. The Lay Wel project: Welfare implications of changed in production systems for laying hens. World's Poult. Sci. J. 63:101-114.
10. Castillo, C., M. Cuca, A. Pro, M. Gonzalez, and E. Morales. 2004. Biological and economic optimum level of calcium in white Leghorn laying hens. Poult. Sci. 83:868-872.
11. Chan, C. & Moran Jr, E. (1985). Egg characteristics of high-performance hens at the end of lay when given cafeteria access to energy, protein, and calcium. Poultry Science,64 (9):1696- 1712.
12. Chandramoni, S. B. Jadhao, and R. P. Sinha. 1998. Effect of dietary calcium and phosphorous concentrations on retention of these nutrients by caged layers. Br. Poult. Sci. 39:544-548.
13. Clunies, M., Etches, R.,Fair, C. &Leeson, S. (1993) .Blood intestinal and skeletal calcium dynamics during egg formation. Canadian journal of animal science,73 (3): 517- 532.
14. Cufadar, Y., Olgun, O. &Yildiz, A. (2011). The effect of dietary calcium concentration and particle size on performance, eggshell quality, bone mechanical properties and tibia mineral contents in moulted laying hens. *British poultry sciece,* 52 (6): 761- 768.
15. De Witt, F., Kuleile, N., Van Der Merwe, H. & Fair, M. (2009). Effect of limestone particle size on egg production and eggshell quality of hens during late production. *South African Journal of Animal Science,* 39 (5): 37- 40.
16. Elaroussi, M. A., L. R. Forte, S. L. Eber, and H. V. Biellier. 1994. Calcium homeostasis in the laying hens. 1. Age dietary calcium effects. Poult. Sci. 73: 1581- 1589.
17. Frost, T. J. and D. A. Roland, Sr. 1991. The influence of various calcium, and phosphorous levels on tibia strength, and eggshell quality of pullets during peak production. Poult. Sci. 63: 339- 343.
18. Garlich, J., J. Brake, C. R. Parkhurst, J. P. Thaxton, and G. W. Morgan. 1984. Physiological profile of caged layers during one production year, molt and postmolt: Egg production, eggshell quality, liver, femur, blood parameters. Poult. Sci. 63:339-343.
19. Guesdon, V., A. M. H. Ahmed, S. Mallet, J. M. Faure, and Y. Nys. 2006. Effects of beak trimming and cagedesign on laying hen's performance and egg quality. Br. Poult. Sci. 47: 1-12.
20. Haugh, R. R. 1937. The Haugh unit for measuring egg quality. US Egg Poult. Mag. 43: 552- 573.

21. Jiang, S., L. Cui, C. Shi, X. Ke, J. Luo, and J. Hou. 2013. Effects of dietary energy and calcium levels on performance, egg shell quality and bone metabolism in hens. Vet. J. 198: 252-258.
22. Keshavarz, K. and S. Nakajima. 1993. Re-evaluation of calcium and phosphorus requirements of laying hens for optimum performance and eggshell quality. Poult. Sci. 72:144-153.
23. Koreleski J, Swiatkiewicz S. 2004. Calcium from limestone meal and grit in laying hens' diets –effect on performance, eggshell and bone quality. J. Anim. Feed Sci., 72:1510-1514.
24. Leeson, S., J. D. Summers, and L. Caston. 1993. Response of brown- egg strins layers to dietary calcium or phosphorous. Poult. Sci. 72:1510-1514.
25. Narvaez- Solarte, W., H. S. Rostagno, P. R. Soares, L. F. Uribe- Velasquez, and M. A. Silva. 2006. Nutritional requirement of calcium in white laying hens from 46 to 62wk of age. Int. J. Poult. Sci. 5:181-184.
26. NRC. 1994. National Recommendation Council, Nutrient requirement of poultry, 9th edition, National Academy Presss; Washington, DC, USA.
27. Olver, M. D. and D. D. Malan. 2000. The effect of choice- feeding from 7 weeks of age on the production characteristics of laying hens. S. Afr. Anim. Sci. 30: 110-114.
28. Ousterhout, L. E. 1980. Effect of Dietary Available Phosphorous and Phytase Level on egg weight and eggshell quality in laying hens. Poult. Sci 59:1480-1484.
29. Pelicia, K., E. Gracia, C. Mori, A. B. G. Faitarone, A. P. SILVA, A. B. Molino, F. Vercese, and D. A. Berto. 2009. Calcium levels and limestone particle size in the diet of commercial layers at the end of the first production cycle. Rev. Bras. Cienc. Avic. 11:87-94.
30. Roberts, J. R. 2004. Factors affecting egg internal quality and eggshell quality in laying hens. J.Poult. Sci. 41:161-177.
31. Roland, Sr., D. A. 1988. Research note: Egg shell problem: Estimated of incidence and economic impact. Poult. Sci. 67: 1801- 1803.
32. Roland, Sr., D. A., M. M. Bryant, and H. W. Rabon. 1996. Influence of calcium and environmental temperature on performance of first cycle (Phase I) commercial leghorns. Poult. Sci. 75:62-68.
33. Safaa HM, Serrano MP, Valenica DG, Frikha M, Jimenez- Moreno E.2008. Productive performance and egg quality of brown egg laying hens in the late phase of production as influenced by level and source calcium in the diet. Poultry Sci. 87: 2043-2051.
34. Song, K.T., Choi, S. H. and Oh, H.R. (2000). A comparison of egg quality of Pheasant, Chykar, Quail and Guinea fowl. Asian- Australia Animal Science13(7): 18-22.
35. Stadelman, W.J. (1977). Quality preservation of shells eggs in egg science and technology (2nd editon) (Ed. W.J. Stadelman and O.J. Cotterill) AVI Publishing Company Inc. Westport, Connecticut, pp41-47.
36. Swiatkiewicz S., Arczewska- Wlosek A., Krawczyk J., Puchala M., Jozefiak, D. (2015). Effects of Dietary Calcium Sources in laying hens' diets with different Ca concentrations. Arch. Anim. Breed., 58,301-307.
37. S. H. An[1], D. W. Kim[2,] and B. K. An*(2016) Effect of dietary calcium levels on productive performance, Eggshell quality and overall calcium status in aged laying hens. Asian Australas. J Anim. Sci. vol 29, No. 10: 1477-1482.

Table 1 Ingredient composition of experimental diet Level of calcium

ITEM	3.8	4.0	4.5
CORN	42g	42g	42g
WHEAT	10g	10g	10g
SOYABEAN MEAL	40g	41g	42g
OAT	5.4g	5.4g	5.4g
CALCIUM AND VITAMIN D_3 TABLET	3.8g	4.0g	4.5g

Table 2 Analysed nutrient composition of formulated diet Level of calcium

Composition (%)	3.8	4.0	4.5
Moisture	7.0005	7.0002	7.0007
Crude protein	0.139	0.137	0.140
Crude fat	81.0000	81.0960	81.0969
Calcium	39%	40.09%	40.56%
Manganese (II) oxide	0.356%	0.355%	0.357%
ZnO	0.257%	0.257%	0.259%
Br	169.4ppm	169.6ppm	169.6ppm
SiO_2	3.034%	3.034%	3.034%
P_2O_5	10.285%	10.285%	10.286%
K_2O	30.775%	30.775%	30.776%
Fe_2O_3	3.626%	3.626%	3.626%
Cl	0.828%	0.829%	0.827%
CuO	607.3ppm	607.2ppm	607.3ppm

TABLE 3 Effect of grades levels of dietary calcium on production performance in the aged laying hens Level of Calcium

ITEM	CONTROL	3.8	4.0	4.5	MEAN ± SE
Feed intake (g/d/bird)	100.2	101.8	100.1	102.4	101 ± 0.57
Egg production (%)	75.1	76.0	75.2	79.1	76 ± 0.93
Egg weight (g/egg)	54.68	54.79	54.82	55.19	54.87 ±0.11
Cracked egg (%)	3.6	3.4	2.3	2.2	2.64 ±0.38

A significant (P<0.05) decrease in no of cracked egg as dietary calcium increases.

TABLE 4 Level of Calcium

ITEM	CONTROL	3.8	4.0	4.5	MEAN± SE
Eggshell thickness	0.36	0.38	0.39	0.43	0.39±0.01472
Dry egg shell weight	5.46	5.49	5.52	5.57	5.51±0.023452
Haugh unit	86.32	86.87	88.59	91.24	88.25±1.105441

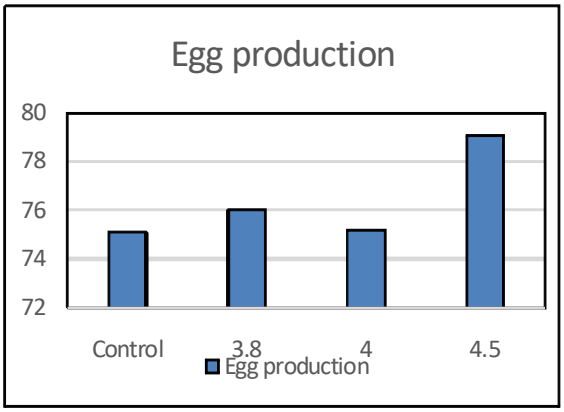

Fig 1 : Egg Production

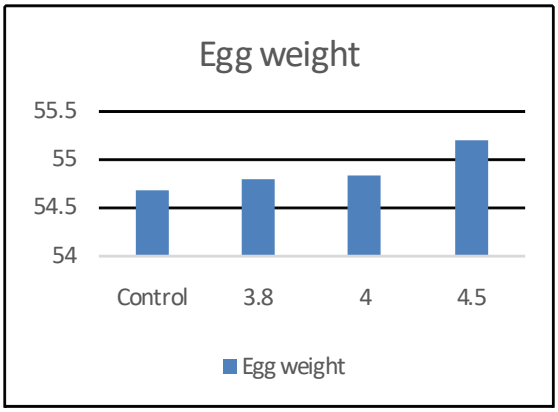

Fig 2 : Egg Weight

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RESEARCH ARTICLE

Analysis and Prediction of Upsurge in Cyclogenesis over Arabian Sea Fabric

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ABSTRACT

Cyclonic Storms (CS) in North Indian Ocean including Bay of Bengal and Arabian Sub-basin are generically formed due to sea surface temperature anomalies and influenced by systems like Nino's, El Nino Southerly Oscillation, Indian Ocean dipole, Intra-seasonal Oscillations, Shamal winds and Makaran Swells. The players for Cyclogenesis are strong wind, pressure drop, storm surges, dust clouds, westerlies and heavy rainfall causing damages like fatalities, pecuniary losses and coastal geo-bio systems. The frequency, amplitude and intensity of CS in Arabian Sea (AS) basins have been increased from 2015 onwards with unprecedented rise in the year 2019 and a tendency of shifting landfall to the countries like Arabia and Somalia. Further, drought prone Somalia state has received two cyclones in a year for the first time. The hike inintensified cyclonic storms in AS basin is the scope of the present study. Data of various cyclones during 1891-2019 has been collected and analysed. It reveals that Indian Ocean dipoles, Intra seasonal oscillations are the favourable conditions for formation, intensification and dissipation of cyclonic storms. Using predictive modelling techniques, it shows that there is a tendency of increase in intensified cyclonic storms over AS basin in next decade. The study concludes that the impact of increase in frequency and intensity of cyclones shall bring greenness to dessert and drought prone countries like UAE, Oman, Yemen, Somalia, and Ethiopia.

Keywords: Arabian Sea; Cyclogenesis Upsurge; Cyclone Prediction; El Niño Southern Oscillation (ENSO).

INTRODUCTION

Cyclones are oceanic disturbances around a deep low-pressure area. The North Indian Ocean (NIO) cyclones are frequent annual occurrences in Bay of Bengal (BoB), but less common in the Arabian Sea (AS). Arabian Sea floor has been divided into six sectors south east (SE), south west (SW), east central (EC), west central (WC), north east (NE) and north west (NW) and the total area comprising of 3862000 km2, maximum width 2400km and optimum depth 4862m (Wikipedia). The countries that encompass the Arabian sea with approximate coast line are India (2500km), Maldives (1000km), Pakistan (1050km), Iran (50km), Oman (1000km), Yemen (500km) and Somalia (100km) depicted in Fig. 1. The cyclonic disturbances in NIO are compartmentalized as Low Pressure area (LPA), Well Marked Low (WML ≤31kmph), Depression/Deep Depression (D/DD ≤51-62kmph), Cyclonic Storms (CS≤ 63 – 88kmph), Severe cyclonic storm (SCS≤ 89-117kmph)), Very severe cyclonic storm (VSCS≤ 118-165kmph), Extreme severe cyclonic storm (ESCS≤166 -220kmph) and Supper Cyclonic storm (SuCS≥ 221kmph) and based on sustained wind speed (3mnts average SWS).

The NIO generates an average 7% of total storms formed annually in the globe according to Kathryn Hansen[1]. There were 1584 number of depressions and disturbances above depression, out of which 102 were during 1891-1899, 1297, were in 20th century, and 186 were during 2000-2019, with a total average of 10 CDs/year. But in Arabian Sea, the yearly average frequency of CD's has been raised from 1 to 1.7 with 8 CDs in the year 2019 (IMD data updated). In 2019, tropical CDs were 143 in entire globe, out of which an average of 105 CDs were intensified to CS and above.

2nd Set Of Nomenclature of CS

The Regional Meteorological Centre (RSMC), IMD, India and five Tropical Cyclone Warning Centers (TCWC) with acceptance of WMO has notified2nd set nomenclature of169 names (13 WMO/ESCAP countries x 13 names each)decided consensus at Myanmar released on 28.4.2020 the upcoming CS's in NIO. The list of old names wasexhausted and was given by only 8countries from 2004. The new countries added at present are Iran, Quarter, Saudi Arabia, UAE, and Yemen. The list of namesupto 1-91 is given in Table 1

Motivation for Study

The following abnormal brewing of cyclogenesis has motivated the study to analyze and predict the unusual meteorological events in the AS floor.

The 21st Century Storms in Arabian Sea

As per records of AS cyclonic storms, prior to Kyarr, the devastative ESCS in AS were AS 03A (Gujarat, 1998), Gonu (Gulf of Persia, 2007), Keila (CS, 2011), Murjan (CS, 2012),Naunak (CS, 2014), Nilofar (VSCS, 2014),Ashobaa (CS, 2015), Chapala (ESCS, 2015), and Megh (ESCS, 2015), Vardah (CS, 2016), Mekunu (ESCS, 2018), and Luban (VSCS, 2018). There was no CS during period 2013-2017 in AS. The AS basin had combated six CSs and above in the year 2019 alone and was first time since 1891. The year 2019 was one hyperactive tropical cyclone season for NIO, particularly the AS basins. But most of the cyclones in AS in NIO form between April to December, with the two frequency peaks one in May and the other during November and strike West coast of India, Pakisthan, and east coast of Arabia[2].

The Miracle in Arabian Sea and WIO 2019

Two set of parallel storms were found in the Arabian Sea and adjacent West Indian Ocean during early December, 2019 clearly indicating climatic change (CC) anomalies in Indian Ocean as in Fig.2. The consequences of the series indicate that the Pak-Arabia dust clouds in Arabian Peninsula tend to drive away the series of disturbances in AS of NIO and WIO. The heavy rain wasresulted in the basin and had floods in

rivers; brought greenness and vegetation to Arabian states. If the CC persist for few years, that may bring a dramatic change in the deserts of Arabia.

LITERATURE REVIEW

There is a gradual declining trend in monsoon activity in BoB[3].The cyclogenesis of CS in tropics are dependent upon Coriolis force (f), +ve relative vorticity at low-level (ζr), vertical wind shear at low tropospheric (Sz), heat content (E) when SST >26.50C, the threshold, atmospheric instability between sea surface and troposphere at 500mb(Δθe), and RH(mid troposphere[4]. Significant increase in frequency of CS in NIO has increased due to rise in SST in NIO including west Arabian Sea in global CC[5].The numbers of CS formed in NIO were 1108 CS, (1885-2009), out of which 68% (751 numbers) slammed 7500km Indian coasts, 19.31% (214 nos) crossed Bangladesh, 5.68% (63nos) landfall Myanmar[6]. The busiest basin is the West Pacific ocean that brewed the highest numbers of typhoons i.e. 26 (tropical CS) and average 16.5 typhoons/year whereas NIO has in average 4.8 CS and above per year[7]. The pre-monsoon storms (AMJ months) are influencing the early/late arrival of SW monsoon whereas the post-monsoon cyclones (OND months) cause more post-monsoon cyclones to brew in AS than BoB. Unlike BoB basin, the CS brews in AS basin during pre and post monsoon period but rarely during monsoon seasons. The devastating tropical cyclones that landfall in Bombay to Gujarat coast in years were 1882, and 1975[8], [9], [10].Cyclones of 1998, 2019 and probability of landfall near Mumbai city is less but storm surge shatters the metropolis due to its low lying topography, large coastal facing, and thick population. AS is less prone to CS but is in increasing trend and 64% of the storm risk is due to anthropogenic activities and CC based on the carbon foot print[11]. The Tropical Cyclone activities are least fluctuating in frequency, duration, intensity, ACE (accumulated cyclonic energy), and PDI (power dissipation index)[12], [13]. The inland onshore landscape playspivotal role in saving the extent of storm surge submergence[14].

METHOD AND METHODOLOGY

Method of Cyclogenesis

Cyclogenesis is not spontaneous under promotive conditions. All CDs do not intensify to CS and some CSs are dissipated within sea. LOPAR, the ab initio cyclonic disturbance, forms only when there is UACYCIR (Upper air cyclonic circulation), maximum low level wind vorticity, higher SST, high RH value, and the clouds should be organized in the deep low pressure area under the sustenance of initial convection condition for a long period and grow[15]. The sustainability of a convective system depends upon survival for an adequate period. The survival ability of the initial convection, Rossby radius of deformation Lr is given by $L_r = \frac{NH}{\zeta_r f}$ where ζ_r low level +ve relative vorticity or atmospheric stability; fCoriolis parameter; NBrunt Vaisala frequency; H is the depth of system [4].The dissipating power EDis $E_D = C_D \rho v^3$,where CD drag coefficient depending on sea roughness; ρ density of air mass; υ wind velocity in Km/h [16].Tropical cyclonic storms are aeolian perturbing systems when the peripheral anticlockwise spiral wind exceeds 63kmph and the pressure difference become 6-10hPa in the eye around the storm producing wave heights > 5.5m.

Methodology

Present study is formation of a time series for past occurrences, evaluation of the strength/intensity of the CD's/CS/SCS and above. Analysis of results of GIS, and space based satellite imageries (Geostationary or Polar orbiting satellites), upper air based (Pilot balloon, RSRW, Profiler, Ground Radar, Aircrafts), Surface observations (AWS, ARG, SYNOP, Buoys, Aviation, Ships), collected from various sources like NASA, NOAA, IMD etc. A comparative study of frequency and causes of occurrence for more storms in AS basin is studied. Statistical studies of the time series are made for both decadal, intensity and frequency. The causes of formation

and propagation under different inducing strategies are explored including the prominence of CD's in the AS basin for last 4-5 years and predictive model to forecast for future frequency, intensity and magnitude in AS.

Data Analysis

Storm statistics over AS Basin

The IMD data for the cyclonic disturbances (CD's) over AS basin is available for the period 1891 to 2019 for 129 years. It is observed from time series that the cyclonic disturbance season starts from the month of May and ends during middle of December in past. From the decadal data series,it is found the mean and standard deviation of for CD's, CS and higher order storms (≥SCS) are 20.5, 11.76 and 6.08 respectively whereas the corresponding standard deviations are 10.66, 6.66 and 3.25 respectively. The status of various storms is given in Fig.3. The data reveals that highest numbers of CDs and CS in AS were in the decade 1891-1899 (45 numbers),2nd highest during 1970-79 (34 CDs), and the 3rdhighest during the period 2010-19 (31 CDs). In comparison, the highest number of devastative CSs were in the decades 1891-99 (28 nos.) followed by the decade 2010-19 (19nos). For SCS and above the numbers are in reverse and the highest was the decade 2010-19 (12nos), 2ndpeakin 1970-79 (11nos) and the 3rd highest was during 1900-09 (9nos) indicating trend isincreasing in frequency and intensity.

Surge in Storms in AS basin

The threshold temperature for cyclogeneses of Tropical storms (TS) is ≥27.50C in AS. The BoB is more conducive for TS than the AS though both the basins have land ward extensions. The area of expanse of BoB is less than AS. About 58% of NIO cyclones formed in BoB whereas AS brew 25% only [17]. The landhit of CS formed in BoB is more in ASsince average SST of the AS is highly uneven seasonally and unmatched to the BoB. The causes are variance in IOD (Warm pool), rainfall, strong winds in SW and NE monsoon, Somali current, less flow from inland rivers and upsurge in vertical mixing[18].

Landfall of Storms over AS and AS peninsular coasts

The total numbers of CS (≥ 34kts) that slammed west coast of India formed in Arabian sea between 1891-2019 were 104 numbers out of which most of them were formed between MJJ months. The post SW or NE monsoon CS also brew during OND months in AS. The countries slammed by CS's along the WC are Gujarat of India (≈ 74%) whereas no report received slamming CS along Karnataka coast. The statistics of slamming CSs and above in different coasts are shown in Fig.4and Table 1.

Drivers for Cyclogenesis in AS

SST anomalies over NIO 2019

The cause of SST anomalies (SSTA) in AS are due to ENSO and IOD[18] [19].NOAA has reported that globally the SSTA in AS has increased from 0.33C (2018) to 0.41C (2019) associated with transition from La Nina of 2017/18 to El Nino of 2018/19. Positive SST departures were observed in NIO near equator, Madagascar (SE ridge of equator), Somalia coast and Arabia. The SSTA in AS has been triggered by the underwater volcanic eruption in West Indian Ocean (WIO). The SSTA during 2019 was next to the warmest SSTA after 2016 (0.44C). The land and SST departure from average was recorded highest in June 2019 in ASsince 1880 (140 year)as per NOAA temperature record. The land and SSTA for 2019 was the 2nd warmest period during Jan–June 2019. This anomaly has prompted to initiation and triggering of all the CDs formed in AS to be drifted to east coast Arabia rather than crossing west coast of India and coasts of Pakistan.

Oceanic current anomalies in AS 2019

NIO had been visited by 12 depressions, 11 deep depressions, 08 tropical CSs, recorded 6 SCSs , 3 ESCS's, and one SuCS (Kyar) which is the highest in terms of intensified TCS and maximum number of TCs in Arabian Sea

than ever recorded. The NIO had experienced Positive Indian Ocean Dipole (PIOD)from June, 2019. Globally, the oceans are heated by average 10 C and some pockets are doubled. The oceanic wave pattern has changed. The oceanic current during Sept-Dec-2019 was prominent. The monthly wave pattern of AS were observed from the data of ASOG/EPSA, SAC, ISRO.The POID in AS influenced the ocean circulation and the trade winds to become intensely warmer than normal SST which has recurrence after 1902 (117years) (IMD). The west part of basin became warmer and eastern chunk became cold than the normal. The setting triggered the convection configuration which invited more rain and CD's in the AS.

Oceanic Niño Index (ONI)

The Oceanic Niño Index (ONI) is one among the popular standard tool to predict El Niño (warm phase), La Nada (normal) and La Niña (cold phase) occasions in the Pacific area in tropics (valid within 50 N-50 S Lat. to 120W-120W Lat). in the tropics/subtropics. It is evaluated trimesterwise considering monthly average SST (≥ + 0.5o C glitch for El Niño), (≤ -0.50 C variance for La Niña) for 5 consecutive 3 months. Nino's and Nina's are SST anomalies for minimum consecutive trimester are weak El-Nino (+ 0.50 C to 0.90 C), Moderate ((+1.00 C to 1.40 C), Strong (+1.50 C to 1.90 C) and Very Strong (≥ 2.00C) [37].

IOD (Positive and negative)

The year 2019 is the highest Indian Ocean dipole (IOD) yearas per Dr Saji N Hameed,the discoverer of the event[20]. The IOD-induced fluctuations occurs in equatorial SST, SL pressure. IOD reforms the north AS winds which form grounds for intra-annual variation in the tropical wave system and climate over east zone of AS [17]. Constant fluctuations in SST of the tropics/sub tropics in WIO and EIO drives CC's as the (IOD) which occur in an average of 10years interval. It is called the Niño of the Indian Ocean. The heat sources that changes the SST of Indian Ocean. Temp. change of (> + 0.50 C) anomaly is pIOD (positive IOD) and < -0.50 C as nIOD (negative IOD) in India. The IOD phenomenon start with pre-monsoon (MJ months),ends during ND months and optimum during SW- monsoon period. The IOD stimulate climate changes like flood, drought, vegetation, rainfall, public health. CD's from east to West in NIO, BoB and AS basins. A pIOD results hot and wet climate in western part of NIO whereas the east zone of NIO is hot and dry[8], [9], [21],[22].

Intra-Seasonal Oscillations (ISO)

About 60% of CS formed in NIO can be linked with intra-seasonal oscillation (ISO) events and during seasonal transitions i.e. (months of AMJ and OND). Two types of ISO are identified i.e. Madden Julian Oscillation (MJO) and Boreal Summer Intra-seasonal Oscillations (BSISO). [23],[25]. The proxies for MJO/ BSISO are RMM-1 and RMM-2 (Real-time Multivariate MJO)[24].The newly developed bimodal ISO index JRA-55 include the MJO and the BSISO indices by applying OLR (outgoing longwave radiation) using EEOF (extended empirical orthogonal function) can be applied to OLR which forecasts the growth of CS in tropical ocean fabric[26].

Maiden Julien Oscillation

The MJO (Madden-Julian Oscillation, 1972) is a moving tropical trimonthly relapse event of disturbances associated with E-ly movement of pressure anomalies, wind, cloud, and rainfall with optimal peaks over EIO, WPO and south of maritime continents (SMC). The harmonic oscillatory motion, reach NIO in its Phase 2 and Phase 3 out of total 8 phases. MJO can have extra-tropical forcing, uncharacteristic cyclogenesis of higher strength as per the graphical analysis of the data from Aug-Sept 2019; Source NOAA/OAR/ESRL,PSD. From the data it is observed that the MJO in AS started in the end of May 2019 set to be very strong[27]

Boreal Summer Intra-seasonal Oscillation (BSISO)

Like MJO; the BSISO-1 and BSISO-2 (Boreal summer intra-seasonal Oscillation) are the prominent northerly moving systems undergoing a strong seasonal variation from Indian Ocean (IO) to West Pacific Ocean (WPO). They play crucial role in deciding CD/CS events in the northern hemisphere. The four responsible factors for

cyclogenesis in NIO are absolute vorticity in lower-troposphere, potential intensity, vertical shear, and relative humidity of mid-troposphere. The BSISO activity monitored since 2013 and forecast as per the BSISO built numerical models and has been presented by the APCC (APEC climate centre)[28], [29] and [30]. About 70% of intra-seasonal cyclogenesis are brewed and favoured for intensification due to northerly transmission of BSISO during intra-transition period of SW monsoon (AMJ and SON months) and rest 30% are due to Easterly movement of MJO activities during post SW monsoon[31].

The low level and over stay of ITCZ

The ITCZ (Intra-tropical Convergence Zone) is normally a band of LPA that hover near equator and within the tropics and cause dynamic thunder storms. ITCZ play vital role in intra-transfer of energies between the northern and southern trade winds. There activities can influence cyclogenesis both in BoB and AS basins. By end of November, the ITCZ normally shift to the S- Hemisphere. In 2019, till 5thDec 2019, the ITCZ was active and was near the equator within N- hemisphere and triggered by the action of PIOD. The month and shifting of MJO phase II has also had favoured cyclogenesis near Sri Lanka and Camorine area in NIO for the storm Pawan and the disappeared storm Seven.

Cyclones in Arabia & Somalia

The favourable conditions for intensification of the CD in AS are high SST, tropospheric CYCIR in the upper atmosphere, high RH. Warm air received from the African and Oman coast add to the cyclogenesis processes in AS. AS basin is prone to strong superficial cooling, more vertical mixing that delimits intensification of cyclones. About 28°C as SST is the limit favourable for convective cloud formation which is satisfied frequently in the BoB Basin but rarely in AS basin. The Arabian Peninsula (Arabia) is a part to West Asia close to Africa. Though Somalia, have the eastern most coast of Africa, had never reported strong CS from Arabian Sea which is neighbour to Arabia. But from 2013, report of one deep depression during 2013, the CS 'Sagar' in 2018 and two CS in 2019 ('Kyarr' and 'Pawan') has indicated that the AS storms are tending to head towards SW Arabian Sea in the 21st century. This tendency shall bring better rainfall and greenness to Arabia, Somalia and Ethiopia.

Summary of climatic events over AS

The major cyclogenesis influencing factors are ENSO, IOD and MJO in the tropical Ocean. The number of CDs, CS, SCS and above were considered from 1975 till 2019 along with the meteorological events like Nino's, IOD and ISO. It is observed that the most favourable threshold for formation of Cyclonic disturbances in Arabian Sea are under El-Nino prevalence, and in PIOD with moderate to strong MJO conditions (Table -2).

Prediction of Cyclogenesis in AS

MATERIALS AND METHODS

The study uses cyclogenesis data of 129 years starting from 1891 to 2019 based on Indian Meteorological Department publications and Wiki data. Three time-dependent observations such as CD, CS, SCS are considered for prediction. Machine learning approach that is widely used for classification and prediction is preferred over traditional ARIMA (Auto Regressive Integrated Moving Average). WEKA, a popular software tool for application of machine learning algorithms is used. It provides an easy-to-use interface for time series forecasting with configuration options for number of time units to forecast and skip list that indicates time period not to consider as increment among others. Linear Regression (LR) and Sequential Minimal Optimization Regression (SMOreg), two well-known algorithms for multivariate time-series forecasting problem are applied on the data. SMOreg is based on support vector machine and supports both linear and nonlinear regression models. Both the regression algorithms are set to its default configurations. Linear

Regression uses Ridge regression to avoid over-fitting and SMOreg uses Normalized PolyKernel as nonlinear kernel function.

RESULTS

The prediction results are show in Fig.5 and Fig.6 at 95% confidence level. RMSE (Root Mean Squared Error) is taken as evaluation parameter to assess the accuracy of prediction. A value of RMSE closer to zero indicates better prediction. The RMSE values of both the algorithms for 11 steps ahead (2020-2030) are plotted in Fig.7. Both the algorithms show error values less that 1.5 which indicates better fitting of regression lines. The algorithm SMOreg shows lower error values for CD, CS and SCS compared to that of LR at initial steps. The error difference gradually reduces as it proceeds towards the end step. Overall, it shows that the SMOreg is better in prediction of cyclogenesis given the dataset at hand.

DISCUSSION

The NIO Basin was hyperactive during the year 2019 by brewing 12 cyclonic disturbances (8 were CS and above) whereas normal it was2/year (1.7 numbers). The CDs in AS basin generally form in SE region basin in the months of May (Pre monsoon). But during post monsoon (Oct-Dec),they were less, in East Central zone. During the month of June, the CD's propagate WNW-ly and recurve NE-ly to cross Gujarat coast in general. Some of them move NW-ly slam coasts of Pakistan, horn of Africa, Oman and Yemen. Sometimes storms hitting south of east coast of India, cross the southern Indian peninsular land mass and enter AS and intensify later to an active system. From 1985 onwards, the incidence of annual rainfall events in Arabia is observed due to shielding effect of the dust cloud The cyclogenesis is initiated in ASwhen SST is (>280 C), strong wind shear, additional influx from surroundings (from WIO).The level of thermal transfer in AS at the interface of SST and Upper Air is high. Cyclogenesis is higher during pre and post monsoon period due to ITCZ positioning, trade wind anomalies and positioning of westerly disturbances.

The less numbers of storms in AS in past years were due to more area, less values of SST and lesser initiating mechanism like IOD, El-Nino ENSO activities, MJO effect and anthropogenic causes. Normally AS brews one SCS, VSCS or ESCS category in 4-5years. In 21st century there were eight ESCS indicating an increasing trendof CS activity along west coast of India. The basin has witnessed 3 CS in 2018 and six during 2019. Previously Saurastra region and the Gujarat coast was the target for land fall, but recent years even Kerala and Karnataka coast are hit by AS cyclonic storms. The confronting causes are: Factors increasing the probability of TC's in the post-monsoon period in AS basin are oil well fire, oil spill in the ocean, concrete jungle in Arabia and increase in GHG gases[32]. The submarine under water volcanic eruption near the Mayotte islandnear Madagascar in adjacent WIO are observed from Nov-2018 accompanied by frequent mild tremors (recorded by the National Centre for Scientific Research (CNRS) in France, the IPGP). The rise in SST can be due to these volcanic eruption can be causes for increase of SST in NIO and brewing intensified storms during 2018 and 2019.
ACE (the accumulated cyclonic energy) was recorded by NOAA as 54 to 88.6 units (10 -1 knots2)with very high kinetic energy during 2019 in comparison to long term average 19.1unit in NIO which has surpassed 2007 ACE highest of 46.1unitsmay be cause forSuCS,Kyarr development in 2019.

The climate change and global warming are the present reflection in positive temperature anomalies (about 10 C averaged) in the AS basin driving more and more intensified CDs. A pseudo El-Nino called El-Nino Modaki as reported by scientists of NIO, Goa is hindering barring BoB basin from brewing CDs. As a result large convergence zone is formed over AS basin to conceive more CS during years of El-Nino Modoki also.
Most of the storms originating in China sea or Bay of Bengal and propagate to south Indian land mass and enter AS basin being less reinforced and further intensify in AS.

Fresh water is lighter than salty water which make layer during stratification. The BoB is lighter and less saline than AS. The higher SST and warm water (less saline) supported formation of TCs in AS. The PIOD is the significant contributor for CD formation over AS during in late-May or early June in 2019 and became abruptly strongly +ve causing high SST. The warm water in WIO and cooler water in Eastern AS may be the main contributor for brewing of storms in AS in 2019. The cyclogenesis prediction results show that there in a continuing increasing trend in cyclonic disturbances, cyclonic storms and severe cyclonic storms over AS basin may increase for the next decade

CONCLUSION

The Arabian Sea basin has turned to be hyperactive with respect to cyclogenesis from 2015 onwards. The age old annual frequency of cyclones has been changed from 1.0 to 1.6 during last 4 years over AS basin. The predictive models have also reiterates the same trend and shows that it will continue during the next decade. The increase in cyclogenesis over AS basin and trend of rising landfall in Arabia, Somalia and Ethiopia will bring more rain to these countries. It is expected that its impact will result more greenness in this region.

REFERENCES

1. Hansen K. Cyclone Hikaa hits Oman, Report from NASA, 24th Sept 2019, available at https://earthobservatory.nasa.gov/images/145645/cyclone-hikaa-hits-oman
2. Wahiduzzaman M. Oliver Eric C. J., Wotherspoon S. J., HolbrooN. J. A Climatological Model of North Indian Ocean Tropical Cyclone Genesis, Tracks and Landfall.Climate Dynamics 2017:49: 2585–2603. https://doi.org/10.1007/s00382-016-3461-4 Hansen K. Spate of Cyclones in the North Indian Ocean, November 7, 2019, available at https://earthobservatory.nasa.gov/images/145841/spate-of-cyclones-in-the-north-indian-ocean
3. Shanas P. R., Sanil Ku. V. Temporal variations in the wind and wave climate at a location in the eastern Arabian Sea based on ERA-Interim reanalysis data. Natural Hazards and Earth System Science 2014:14: 1371-1381. https://doi.org/10.5194/nhess-14-1371-2014
4. Gray, W. M. Tropical cyclone genesis. Department of Atmospheric Science, Colorado State University, 1975.
5. Singh K., Panda J., Osuri K. K., Vissa N. K. Progress in Tropical Cyclone Predictability and Present Status in the North Indian Ocean Region. Recent Developments in Tropical Cyclone Dynamics, Prediction, and Detection, A. R. Lupo, IntechOpen 2016. DOI: 10.5772/64333
6. Tyagi, A., Bandyopadhyay, B. K., Mohapatra, M. Monitoring and prediction of cyclonic disturbances over North Indian Ocean by Regional Specialized Meteorological Centre, New Delhi(India): Problems and Perspective. Indian Ocean Tropical Cyclones and Climate Change, 2010:93-103. DOI: 10.1007/978-90-481-3109-9_13
7. Evan A., Camargo S. J. Climatology of Arabian Sea Cyclonic Storm. Journal of Climate 2011:24(1):140-158 DOI: 10.1175/2010JCLI3611.1
8. Saji, N. H., Goswami, B. N., Vinayachandran P. N., Yamagata T. A Dipole Mode in the Tropical Indian Ocean. Nature 1999:401:360–363.
9. Shaji C., Kar S. K., Vishal T. Storm Surge Studies in North Indian Ocean: A Review, Indian Journal of Geo-Marine Science 2014:43(2):125-147.
10. Sobel A. H., Lee C. Y., Camargo S. J., Mandli K. T. Tropical Cyclone Hazard to Mumbai in the Recent Historical Climate, Monthly Weather Review, American Meteorological Society 2019:147:2355-2366. https://doi.org/10.1175/MWR-D-18-0419.1

11. Murakami H. B,. Wang T. Li, and Kitoh A., Projected increase in tropical cyclones near Hawaii. NatureClimate Change, 3, 749-754, 2013, doi:10.1038/nclimate1890. IPRC-975.
12. Singh O.P., Ali Khan T.M., Rahman M.S., Changes in the frequency of tropical cyclones over the north Indian Ocean Meteor Atmos Phys, 75(1); 11-20; (2000); DOI: 10.1007/s007030070011
13. Bhardwaj P.j, Singh O. and Yadav R. B. S., Probabilistic assessment of tropical cyclones' extreme wind speed in the Bay of Bengal: implications for future cyclonic hazard, Natural Hazards, 10.1007/s11069-020-03873-5, (2020).
14. Murty P. L. N., Rao A. D., Srinivas K. S., Rao E. P. R., and Bhaskaran K. P. Effect of Wave Radiation Stress in Storm Surge-Induced Inundation: A Case Study for the East Coast of India. Pure and Applied Geophysics 2019. https://doi.org/10.1007/s00024-019-02379-x
15. Chand R., Singh C. Relation of Frequency of Tropical Cyclones Over North Indian Ocean and North West Pacific Ocean with Sea Surface Temperature Anomaly Over Nino 3.4 Region and Indian Ocean Dipole. In: Mohapatra M., Bandyopadhyay B., Rathore L. (eds) Tropical Cyclone Activity over the North Indian Ocean. Springer, Cham, Springer, 2017:233-24.
16. Singh K., Panda J., Osuri K. K. and Vissa N. K., Progress in Tropical Cyclone Predictability and Present Status in the North Indian Ocean Region, book: Recent Hurricane Research II: Dynamics, Prediction, and Detection; 2016; Edition: 2nd; DOI: 10.5772/64333
17. Mohapatra M, and Sharma M., Characteristics of surface wind structure of tropical cyclones over the north Indian Ocean, J. Earth Syst. Sci. 124, No. 7, October 2015, pp. 1573–1598
18. Jaswal A., Singh V., Bhambak S. R. Relationship between sea surface temperature and surface air temperature over Arabian Sea, Bay of Bengal and Indian Ocean. Journal of Indian Geographical Union 2012:16(2):41-53.
19. Webster P. J., Moore, A. M., Loschnigg, J. P. &Leben, R. R., 1999, Coupled oceanic-atmospheric dynamics in the Indian Ocean during 1997–98. Nature 401, 356–360 (1999).
20. Saji H., N.; Jin, Dachao; Thilakan, Vishnu (2018), A model for super El Niños, Nature Communications.,9 (1): 2528.on 28th June, Bibcode:2018NatCo...9.2528H. doi: 10.1038/s 41467-018-04803-7.
21. Anoop, T. R., Sanil Kumar, V., Shanas, P. R., Glejin, J., Amrutha, M. M. Indian Ocean Dipole modulated wave climate of eastern Arabian Sea. Ocean Science 2016:12(2):369-378. https://doi.org/10.5194/os-12-369-2016
22. Cai, W. et al. Increased frequency of extreme Indian Ocean Dipole events due to greenhouse warming. Nature 2014:510:254–258.
23. CaiWenju, Wang G., Gan B., Wu L., Santoso A., Lin X., Chen Z., JiaF.,Yamagata T. Stabilised frequency of extreme positive Indian Ocean Dipole under 1.5 °C warming. Nature Communications 2018:9:1419. https://doi.org/10.1038/s41467-018-03789-6
24. Kikuchi K. and Wang B., Formation of tropical cyclones in the Northern Indian Ocean associated with two types of tropical intra seasonal oscillation modes. J MeteorolSoc. Jpn; (2010);88;475–496
25. Mishra S. P., Sethi K. C., Mishra D. P., Siddique M., Pre-monsoon cyclogenisis over Bay of Bengal, Int. Jr. of Recent Technology and Eng. (IJRTE);8(2), July 2019 , 4895- 4908; DOI: 10.35940/ijrte.B3694.078219
26. Kikuchi, K. Extension of the bimodal intra-seasonal oscillation index using JRA-55 reanalysis, Climate Dynamics 2020:54:919-933. https://doi.org/10.1007/s00382-019-05037
27. Gottschalck J., Zhang Q., Wang W.,'Heureux Michelle L., Peng P., MJO Monitoring and Assessment at the Climate Prediction Center and Initial Impressions of the CFS as an MJO Forecast Tool, 2010; https://www .nws.noaa.gov/ost/climate/STIP/CTB-COLA/Jon_042308.html
28. Emanuel, K.A. The power of a hurricane: an example of reckless driving on the information superhighway. Weather 1998:54:107-108.
29. Emanuel K. A., and Nolan D. S. Tropical cyclone activity and global climate. Proc. 26th Conf. on Hurricanes and Tropical Meteor., Miami, FL, Amer. Meteor. Soc., 2004:240–241

30. Yanase, W., Satoh M., Taniguchi H., and Fujinami H. Seasonal and Intra-seasonal Modulation of Tropical Cyclogenesis Environment over the Bay of Bengal during the Extended Summer Monsoon. Journal of Climate 2012:25:2914–2930. https://doi.org/10.1175/JCLI-D-11-00208.1
31. Kikuchi, K., Wang, B., Kajikawa, Y. Bimodal representation of the tropical intra-seasonal oscillation. Climate Dynamics. 2012:38:1989-2000. DOI 10.1007/s00382-011-1159-1.
32. Guimareas S. O. Climate Models Accumulated Cyclone Energy Analysis, Book: Current Topics in Tropical Cyclone Research, 2020. DOI: 10.5772/intechopen.91268

Table 1.The Decadal Slam Of Cs By Coastal States In Ec; India, Pakistan, Oman, Yemen And Somalia.

Year	Cyclonic storms land slamming Arabian sea (East &West coast) ≥34kts or ≥ 63kmph							
	EC-Pakistan	EC-Oman	EC-Yemen	EC-Somalia	WC-GuJa	WC MH/Goa	WC-Karnataka	WC-Kerala
1890-1899	2	1	2	0	4	0	0	0
1900-1909	2	1	2	0	1	0	0	0
1910-1919	0	2	0	0	1	0	0	0
1920-1929	0	3	0	0	1	0	0	1
1930-1939	0	0	0	0	2	0	0	1
1940-1949	2	1	0	0	3	3	0	0
1950-1959	0	3	0	0	0	0	0	0
1960-1969	2	4	1	0	2	2	0	0
1970-1979	0	5	4	0	2	0	0	0
1980-1989	1	1	1	0	3	0	0	0
1990-1999	3	4	1	0	3	0	0	0
2000-2009	5	2	0	0	0	1	0	0
2010-2019	2	8	5	2	2	0	0	0
Total CS	19	35	16	2	24	6	0	2

Table 2: The Status Of Cyclogenesis Influencing Factors In As Of Nio (2000-2019)

Year	CD's	CS	SCS	EL Nino	IOD	MJO
	AS	AS	AS	ENSO Type	pIOD/nIOD	Strong/Mod/Weak
2000	0	0	0	WL	Nil	nil
2001	3	3	1	La Nada	nIOD	Mod-weak
2002	1	1	0	ME	pIOD	Strong-Mod
2003	1	1	1	La nada	Nil	weak
2004	5	3	3	WE	Nil	Strong-Mod
2005	2	0	0	WL	Nil	Mod-strong-nil
2006	1	1	1	WE	pIOD	Weak-mod
2007	3	2	1	SL	Nil	Weak
2008	2	0	0	WL	Nil	Strong-weak
2009	3	1	0	ME	Nil	Mod-strong
2010	2	2	1	SL	nIOD	Mod
2011	5	2	1	ML	Nil	Weak
2012	2	1	0	La Nina	pIOD	Mod
2013	1	0	0	La nada	Nil	Weak

2014	2	2	1	WE	nIOD	Weak
2015	5	3	2	VSE	pIOD	Mod
2016	2	0	0	WL	nIOD	Weak
2017	0	0	0	WL	Nil	Mod -weak
2018	4	3	3	WE	pIOD	Mod
2019	8	6	4	WE	pIOD	Mod
WE=Weak El Niño, ME=Moderate El Niño, SE=Strong El Niño, VSE=Very Strong El Niño, WL=Weak La Niña, ML=Mod. La Niña, SL=Strong La Niña pIOD: Positive IOD; nIOD: Negative IOD, NIL: No IOD event						

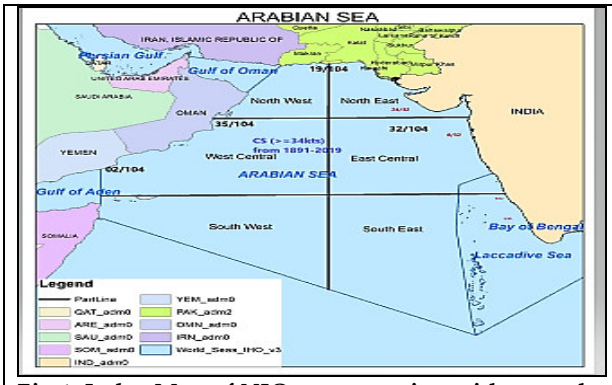


Fig.1. Index Map of NIO segmentation with coastal states around Arabian Sea (AS); Source: Indian Meteorological Department (IMD).

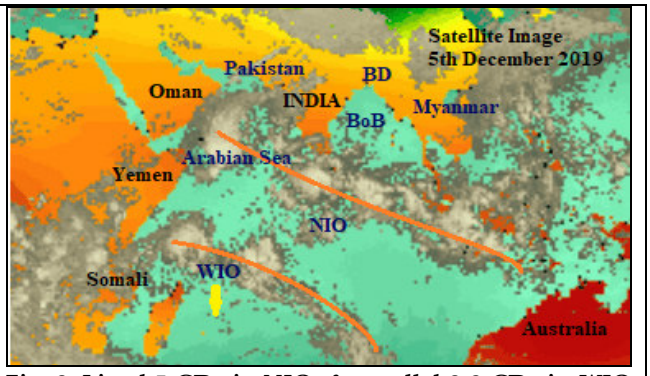
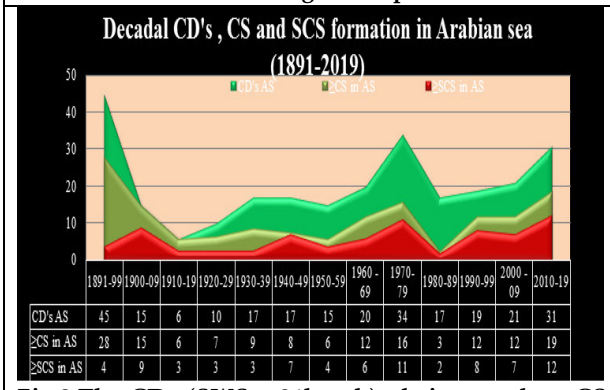


Fig. 2. Lined 5 CDs in NIO, & parallel 2-3 CDs in WIO heading Africa Source: Dremann C. C. [35].



	1891-99	1900-09	1910-19	1920-29	1930-39	1940-49	1950-59	1960-69	1970-79	1980-89	1990-99	2000-09	2010-19
CD's AS	45	15	6	10	17	17	15	20	34	17	19	21	31
≥CS in AS	28	15	6	7	9	8	6	12	16	3	12	12	19
≥SCS in AS	4	9	3	3	3	7	4	6	11	2	8	7	12

Fig.3.The CDs (SWS ≥ 31kmph), their growth to CS (SWS ≥63kmph and intensification to SCS and above (SWS ≥ 89kmph) recorded in Arabian Sea 1891 to 2019;Source: Indian Meteorological Department (IMD).

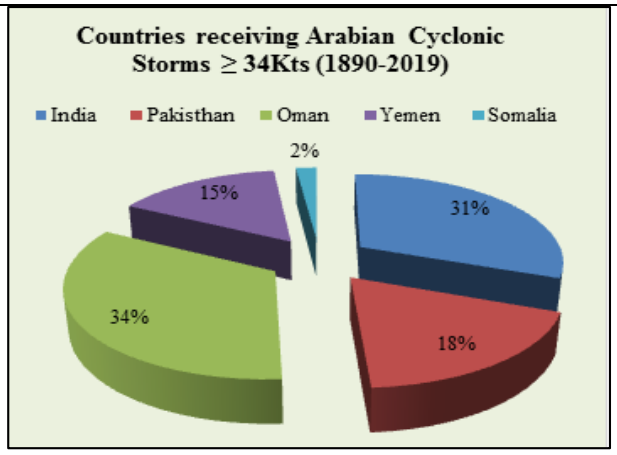


Fig.4. The % of landfall of cyclonic storms by the encircling countries around AS Peninsula

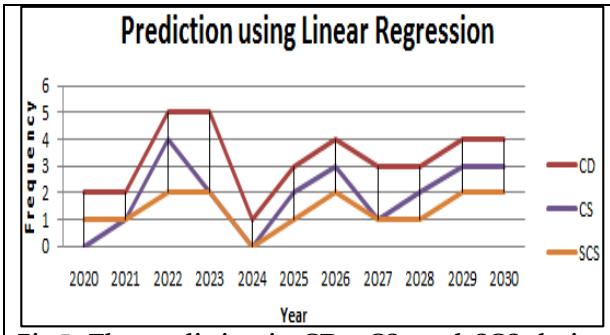


Fig.5. The prediction in CDs, CSs and SCS during 2020-2030 using LR model

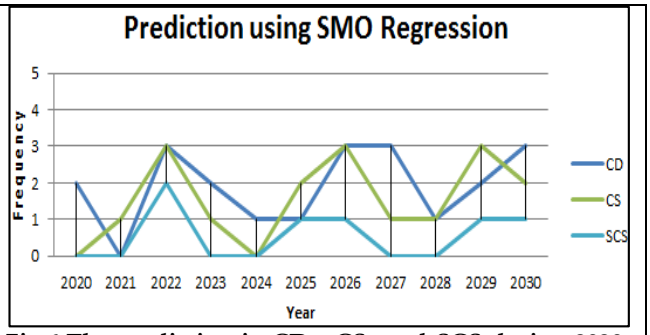


Fig.6.The prediction in CDs, CSs and SCS during 2020-2030 using SMOreg model

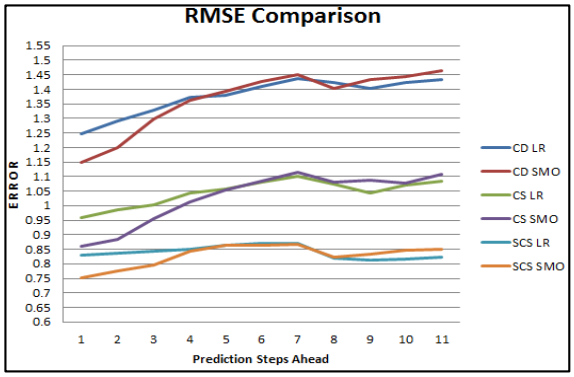


Fig.7. The error comparison of the LR and SMOreg models used for predicting CDs. CSs and SCS in AS basin

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RESEARCH ARTICLE

Disaster Resilient Built Environment in Odisha coast, India

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ABSTRACT

This paper explores the challenges and opportunities for compliance of building ethics for disaster resilient structures, focusing on traditional, informal and present coastal structures along east coast of India, during varieties of cyclonic storms. Since seven years it is observed the frequencies of cyclonic storms in Bay of Bengal has reduced whereas the intensities have abnormally surged up. After the super cyclone 1999, the 480km long Odisha coast has interacted with cyclones above severe cyclones are Phailin (2013), Hudhud (2014), to Fani (2019), Bulbul (2019) and Amphan (2020) have caused enormous damages to the structures, inundation and devastation of the green coast. These cyclonic storms highlights a major problem to existing structures of 20-25km inland and both sides of the storm track as they are non-compliance with safe building codes. In India building codes for disaster resilient structure do exist, but compliance to code is lacking due to cultural, economic and political concerns both in coastal towns and rural areas. Before 2-3 decades; most of the coastal houses are mud built and thatched roof causing less economic losses. But 1970 onwards the tiled roofs, Slant roofs of asbestos and tin causing more trauma and fatalities.Thebuilding code for cyclone resistant structures has become a challenge to the villagers due to their lower resources and weaker governance. Field surveys were conducted in Puri and Bhubaneswar as case studies of post Fani housing. According to local people, the ignorance about the safe building's code for cyclone resilient structures, and poverty are the main cause for their sufferings.

Keywords: Cyclonic storms, Resilient buildings, Odishacoast, DRR, Fani, Amphan

INTRODUCTION

Entire earth is stressed under natural or anthropogenic hazards, meteorological extremes and associated disasters. Unprecedented climate anomalies have escalated the frequency, intensities and magnitude of these disasters. The ecology and the biodiversity are encountering fatalities, damages, and losses to societal, fiscal and political status of

the world. Over the past few decades, a series of meteorological extremes like earthquakes, Tsunamis, cyclonic storms and high floods have shattered several parts of the globe, which have challenged the existing risk reduction, and management system. Disaster can be flood, cyclonic storms, tsunami, drought, lightening, viral diseases, earth quake and landslides etc. Out of the seven natural disasters cyclonic storms are major life taking and devastator. In Indian context; super cyclone (1999), Chobari earth quake, Gujarat (2001), Indian ocean Tsunami (2004), Mahanadi floods (2008 and 2011), Tropical cyclones at Paradip (1999), Phailin (2013), Hudhud (2014), (Titli) 2018 and Fani on 26th April-3rd May and the Bulbul (5th to 10th Nov) in 2019 and Amphan (16 to 21May 2020) are some of the major catastrophes and apocalyptic disasters over the past 20years in India. TheOdisha's coastal territory has been victim to mainly upsetting cyclonic storms having long-term impacts

Disaster risk resilience factors can be categorized into six groups: infrastructural, psychological, socioeconomic, social-capability and social capital, managerial/ organizational, and culturallivelihoodassets.Measuring resilience, the focussed elements are Technical ability, Skills and training levels, pecuniary eminence and progress, environmental quality and natural resource management institutions through Community resilience Chandra et al, 2013[1], Jue-Sheng 2014[2], Patel et al 2017[3]. For immediate help, the state provides expert disaster management officials like the Orissa State Disaster Management Authority (OSDMA) and the Orissa Disaster Rapid Action Force (ODRAF). Present study emphasizes on community coping with structural and non-structural safety aspects in the built environment and proposing methodologies to have strategic planning for resilient buildings in cyclone prone areas affected by Fani, the extreme severe cyclonic storm along Odisha coast.

Cyclone Category

The characteristics of different category of tropical disturbances and cyclones in North Indian Ocean (NIO) according to 3mnts average wind speed are Low pressure Area (LPA; <31 km/h), Depression (D;31 to 49 km/h), Deep Depression (DD;50 to 62 km/h), Cyclonic Storm (CS; 63 to 88 km/h), Severe Cyclonic Storm (SCS;89 to 118 km/h), Very Severe Cyclonic Storm (VSCS;119 to 167 km/h), Extreme Severe cyclonic storm (ESCS; 168 to 221Km/h) and Super Cyclonic Storm (SuCS; ≥ 222km/hour). The categorisation can be varied based upon eye extension, and the pressure dropMishra et al., 2014[4]. The cyclogenesis factors for type of CS may include the storm swale/surge, the travel time and the path of propagation along with seasonal behaviour and the favourable systems associated with the storm like El Nino, ITCZ positioning, OLR and MJO etc. can be a better categorisation(Li z et al., 2019[5]Mishra S. P. 2020[6]).

Objectives

Odishahas a long coast line of 480km; due to its topography is vulnerable to natural disasters like floods, cyclones, droughts, coastal erosions with sinking and shrinking of its deltas. Hence it is the instant need for a coordinated strategic plan for attaining disaster resilience community to risqué the victims affected from disaster management activities. The built up environment play important role in city or village communitybuilding.The resilient building helps to maintain sustainable living and safe life style along the coastal front.It is of paramount importance to develop a built environment with an effective degree of resilience to withstand and adapt to the threats of disasters particularly the most hostile storms along coastal Odisha. The present paper aims to explore the challenges in achieving a disaster resilient built environment within cities/ rural areas to provide recommendations as to how these challenges could be averted.

During Fani and Amphan, the last two cyclones have battered the entire coastal Odisha. As such two case studies were conducted selecting a city, Bhubaneswar; the capital city of Odishaduring Fani and like Bhogaraimany coastal blocksofBalasore to JagatsinghpurdistrictduringAmphanhas been harshly shattered. The data were gathered through semi-structured interviews with the local and other government and NGO officials, policy makers, industry practitioners and experts who are engaged in the respective areas either for restoration and renovation of the distorted infrastructure. In addition, expert interviews were conducted who are extensively engaged in disaster management and built environment of related disciplines to validate the case study findings. The interview data

were analysed based on the findings conclusions are drawn for the challenges associated in achieving a disaster resilient built environment within Odisha.

METHODOLOGY

Disaster resilience and it's management had been considered bitch's affair tried to satisfy the deities by ritual customs in past. Advancement of science and modern structural methodologies has shaped the disaster resilient structures from 20th century only. It was mainly to explain why some communities did better or was successful in responding to and bouncing back from large-scale disasters while others failed. Previous studies have suggested that a community's disaster resilience can be attributed to a variety of factors: a sense of community; problem-focused coping style; self- or collective efficacy; social support or social capital; citizen participation in voluntary Organizations; local leaders; disaster management policies; plans, and practices process- oriented hazard mitigation policies. The organizational preparedness with cooperation learning can protect us from storms. Communication capabilities, indigenous expertise, experiences, significance, and ethos, infrastructure, life lines and the demographic features of a community can ameliorate the impact.From observation and case studies, number of barriers for creating a disaster resilient built environment within cities and rural areas of Odisha are identified. The main challenges related to disaster risk resilient structures of Odisha are discussed with about 50 CS and above in 20th century and above 10 in 21st century till date.

Informal Buildings

Lots of informal buildings and temporary structures like mud built hutments, palm leaf cottages are there in coastal Odisha and even in slums of the city like Bhubaneswar which are
in the coast constructed without basic plans, infrastructural designs and appurtenant facilities. These urban slum dwellers and rural communities are vulnerable to floods and cyclone hits(Fig 1). The affected people and the government pose major challenge to restore, rehabilitate and relocate the disaster oustees. These permanent inhabitants have their livelihood and earning avenues depend upon the means and sources of the neighbourhood areas. These informal building are dilapidated with the gusty spells of the cyclone Fani.The structures made up of barbed fenced earthen houses, thatched roofs, old buildings with deteriorated and weakened conditions of walls, unreinforced or old poorly constructed structures of rural, and slum communities are most vulnerable for storm impactFig 2(a) and 2(b). The topography of land, and temporary shelters in low lying, lacustrine, coastal and isolated areas are also vulnerable to the aeolian forces and whirl wind zones affect the poor structures.

Lack of Regulatory Frameworks

Based on observation it is revealed that the existing regulatory framework on planning, design and construction does not adequately look into the resilience. "Policy for housing for all in Urban areas 2015" the updated Code of practice for design loads for buildings and structures Part 3 is not taken in account. Even the amendments to the Indian standard codes are not updated in policy booklet. Number of initiatives was taken at the state and central level to address all aspects of housing for urban poor including slum rehabilitation, redevelopment as well as new housing and for needy rural community. Maintain the multipurpose disaster resilient building every year not to deteriorate due to salinity Fig 2.The reconstruction/rehabilitation of public damaged houses/villages in-situ should be allowed not to be done beyond the CRZ buffer zone (> 500m from coast line). Reconstruction activities must enforce DRR laws and multi hazard resistant features.

The IS: 875 (Part 3) – 1987[7]has provision for wind pressure at ground elevation is given by $P_z = 0.006 V_z^2$ where $P_z$and$V_z$are the design pressure and wind velocity during heavy wind. The values of $V_z$calculated as per the code.The pressure of wind depends upon flow aero-dynamics circumscribing the buildings, the vertical faces under pressure, the lateral and leeward faces receiving suction, the sloping roofs acting as a barrier. The sun shades and roof projections are also subjected to uplift pressuresVandari et al., of IITKanpur[8].

A model has been designed but not applicable to buildings or structures with unconventional shapes, unusual locations, and abnormal environmental conditions that have not been covered in this Code.as Fig 3 (A) and (B). Designinghazard&risk maps, disaster resilience planning and construction guidelines and set back zones are defined. However, many of these initiatives have not been mainstreamed into building planning and approval process of the local governments and as a result the awareness on these new initiatives was somewhat low with the local level staffs (Block level) who are actually engaged in the building approval process.

Traditional old structures in Odisha have taught us buildings with large openings are vulnerable to cyclonic gusty winds where as a small opening in wall act as a tunnel to equalise the external wind pressure and internal room pressure so that there shall be less suction and lift (Fig 4). The Gujarat State Disaster Management Agency (GSDMA bulletin[9]) have reported a building with large opening of 1.75mx1.2m in a wall can build up wind pressure 0.7 kN/m^2 where as a small opening has low wind pressure 0.2 kN/m^2 . Similarly the old ATTU (a mud roof below the thatching) saves the storm victims from fatalities and trauma and also behaves as a tunnel to normalize building pressure during gusty wind.

Old Building at Risk Infrastructure

A good number of old school buildings, bungalows and houses of zamindaris of heritage are there in many villages of Odisha which were of belated design without adequate consideration to disaster impacts and resilience(Fig 4). Government is taking steps to replace these old buildings and at risk infrastructure. But due to lack of funding all school are not immediately replaced. Strength, durability and performance monitoring is not done periodically. Strengthening of structural members for all old institutional building is not done. Also, poor maintenance of the existing infrastructure intensifies the risk of disasters like falling of walls after heavy storm and rain. Even in 2019 also there are schools without RCC slab. The schools are with dangerous tin and asbestos roof and blows away with CS wind (Fig 5). The connection between these sheets and roof is not adequate to resist wind speed more than 150 KMPH. Also the broken fibres of asbestos after a storm may cause asbestosis, lung cancer etc. Mostly temporary prefabricated structures and Kutchahouses got affected due to Fani. Also inadequate cleaning and maintenance of canals and other natural and man-made rainwater drainage systems has been identified as one of the reasons for recent flooding in the state.

Unplanned Cities and Urbanisation

The meteorological setting is to be accounted for achieving safe and suitable design for dwellings considering the players are temperature, direction and strength of wind and precipitation (*Landsberg H. E, 1976[10]*). Most of the cities in Odisha are unplanned and also a rapid urbanisation is undergoing at present. As a result most of the protective and servicing infrastructure is not sufficient to serve the increasing population. Many dwelling houses and other buildings are built without adequate consideration of disaster risks and vulnerabilities. More recently the state was severely affected by floods and cyclones and the impact was aggregated due to poor design and construction activities in. Some of the major reasons behind the increased impacts of flooding are, filling of agricultural lands, paddy fields and other low-lying areas; obstructing the natural rain water drainages for the construction of houses and other structures; and, blocking natural waterways, blocking of natural drains with plastics, without adequate drainage structures, prevention from percolation of runoff water to ground and increase the surface run off.

Institutional Arrangements

In Odisha, there are a number of governmental organisations eg BDA, BMC, R&B etc responsible for the design, development, operation and maintenance of the built environment. The urban planning in functions is in close collaboration with various agencies under different government ministries. Each of these agencies has a specific role in the process of planning, designing and approval of housing and infrastructure. Accordingly, all these departments are responsible for initiating disaster risk reduction and contribute to building safer cities. In addition, further collaboration is required with OSDMA and technical agencies responsible for producing information related to

natural hazards. All these indicate that there is a system in place to create a disaster resilient built environment in Odisha. However it is witnessed that the current system demonstrates a number of drawbacks such as lack of well-defined roles and responsibilities; overlapping of responsibilities; lack of coordination among organisations; political will and commitment.

Lack of Funding

They have capacity-building programmes at ab-initio level to enact such catastrophes. Disaster resilient built environment is relocating existing vulnerable structures; enforcing resilient building codes and standards; use of hazard resilient designs, specifications, construction methods, materials and technologies; protecting critical infrastructure in the city and constructing protective infrastructure; sustainable urban planning; and land use Practices. All these invariably require a considerable amount of funding for satisfactory completion. Paucity of adequate budgetary provision and alocation is the main challenge for disaster resilient structure in rural community and urban slum areas. The little state Odishais unable to allocate proper funds to combat floods, droughts, cyclonic storms and under lock downs and social distances byvirulentpresent COVID-19 in 2020.

Inadequacy of Qualified Human Resources

Qualified staffs knowledgeable on DRR are limited especially at the local level and as a result some of the resilient measures are overlooked. Local governments are the primary agency in the country for issuing development permits for buildings and lands and issuing certificates of conformity to ensure that the constructions carried out complies with the approved plans. In doing so, all disaster risks and vulnerabilities need to be considered before issuing development permits and the certificate of conformity. However without the adequate number of qualified staff, knowledgeable on DRR, it is difficult to build a resilient built environment and to effectively monitor the development activities carried out in the city. Also the most affected people are from rural community and they are far behind from knowledge of Indian standard codes and their importance.

Inadequate Capacities of Municipal Councils

Municipal councils are the premier form of local governments which are based at the most urban cities of the country. They are the primary agency in the country for providing planning approval for new buildings, alterations and extensions to existing buildings, and changing the use of buildings and land use and issuing certificates of conformity to ensure the construction complies with the approved plan. Thus, municipal councils are required to play an inevitable role in creating a resilient built environment within cities. However, the empirical evidence revealed BMC is facing a number of challenges in its contribution to making a resilient built environment within city. The main issues that have emerged are legal framework; lack of adequate tools, techniques and guidelines; human resource and funding constraints; lack of focus; coordination; managing the long term process; dependence on central government; irregular occurrences of disasters; community actions, leadership and organisational culture; and corruption and political interference.

Awareness for Resilient Structures

Lack of awareness for disaster resilient structures amongst the citizens is also identified as a challenge. Awareness camps should be organized in community level to make them understand that the severity of calamity will be increased in coming years due to climate changes. And for rural community it is better to do investment for climate proof infrastructure may cost a little extra upfront, but it will deliver more sustainable infrastructure in long term. Critical infrastructure should be protected from future climate impacts (OAS/USAID norms[11]) The walling, cladding, wind bracing, ground anchoring and eves must be properly designed to resist sloped structures which are existing in the coastal areas prone to storm, surges and floods(Fig 6)(NDMA guideline[12]). As far as possible flat roofs with light weight concrete structure (with ferro cement) are preferred in disaster prone areas. Four side slanted roofs with small opening is desired in cyclone vulnerable areas (Agrawall A., 2007[13]). The major plantations must

be avoided near the houses except some small fruit bearing trees without large trunks for shading in summer (Lemon, orange, Guava, dwarf coconut, cashew nut trees plantains etc.)

Vulnerable Part of Structure

Rooftops, gables and ridges

They are considered as the most common area of catastrophe during cyclonic storms. It isdue to insufficient thickness, quantity of fastenersand fastening devices. Roofs can be protected by installing hip roofs having pitch ranges within 25^0 to 40^0 .Overhangs either avoid or small length and the separated patio roofs and verandas. The main ridge using gussets, collar ties and metal straps to be secured with proper driving screws (Gibbs et al., 2001[14])

Know foundations and materials: The foundations are sensitive part of the building.Foundation damage, destruct structural walls even increase the risk of the building to detach from foundation. The depth of foundation is to be judged depending upon soil type and bearing capacity. The foundation construction should have proper Knee bracing/ full diagonal bracing with a foundation RCC band. The walls must be built with brick or stone have minimum four bands at DPC level, window sill level, lintel level and below roof level with RCC bracings/ buttresses if required to be pr4ovided in the long walls.Ferro-cement need for the plastering and corner reinforcement need to be provided (Keote S. A. et al., 2015[15]).

Thatched houses: They should be provided with ATTU below roof, with metal strips and nailed at the joints, the bamboo battens well bound with new ropes and the houses must be well fenced with strong shrubs. The rooms have very small openings and must be placed clustered and over open field without large plantations. Large verandas as overhang must be avoided in cyclone prone areas in sloped roof houses.

Tiled buildings: Must have compound walls and the court yard should not have large trees. The over laps within tiles to be jointed with cement mortar. The roofs should be inclined < 25^0 to the horizontal. The tip of the roofs (ridges)should be well designed with gussets/collars or metal strips so that the wind shall pass away over it. The roofs should have strong sal/metal battens jointed with rafters by U-hooks, eaves provision with concrete strips, replacement of rusted bolts, old broken tiles, and metal straps. The strong roof trusses (king and queen posts) should be strongly anchored with walls and the rafters. There should have reinforced concrete bands in the compound walls if needed should be counterfort structures. Hipped roofs are better than slanted roofs during cyclones(Panda and Mishra 2020[15])

Concrete/Prefabricated structures: The roof top should not have large water tanks, poorly structured overhead rooms. The outer walls of prefabricated structures as far as possible should be plastered with light weight (ferro-cement) thin walls over the aluminium cladding and the structure must be well anchored with basement. Openings near corners must be avoided as they are the suction zones for uplifting the structures. Glass or transparent plastic panels are to be avoided(Taher R. 2010[16]). In coastal zones of Odisha the cyclones generally approaches from ESE to ENE. But the wind direction received by the buildings is random as the Aeolian forces are rotating in nature. So the buildings should be well protected from all direction to combat cyclonic wind. It is long practices that the well protected house is square or elliptical shaped rather than rectangular or L-type or T-type but the houses should be zigzagged to dissipate wind energy(Fig 7).

Rebuilding Resilient Structures

Fani has devastated 90899 houses fully damaged, partially damaged 157200 houses as per district administration Puri. These fully damaged houses need urgent reconstruction where a resilient build environment under proper design maintaining safety procedures is highly essential. The model of a luxurious storm resistant structure with concrete roofing or thatched roofing is shown in fig 8

While passing through north Odisha coast, the VSCS Amphan had uprooted trees, inundated paddy fields in the low lying areas. Only some kutcha buildings were damaged there was zero death reported. The 33-KV feeders have been damaged, impacting almost all electricity consumers in coastal districts along the north coast from Balasore, Jagatsinghpur districts.

Cyclone Prone Structures

Foundation: In coastal areas the foundation is important for cyclonic storms in low lying areas due to submergence by storm surges. The points of importance in foundation are elevating the structure above GL to avoid inundation and larger foundation depth. The bracing arrangement is essential if the foundation is piles or can be opted for well foundation.

Super structure: To maintain the structure monolithic and uniformity use same construction type up to full height. Instances of failure have been noticed at the joints of two types of structures. Use good quality construction materials and use fully or partially reinforcement well grouted for structural safety during cyclone. Along with plinth band lintel and extra bond beam may be provided with concrete structures. To avoid common wall connection failure, it can be opted for use of reinforcing bars of masonry walls at the corners Fig….

Disaster Risk Reductionstructural planning:

Old settlements made by past kings in Odisha (Sasan's) are in the valleys and had symmetrical rows planned with a central road and surrounded by coconut, palm and pea nut trees with passages for wind to save the settlement from cyclonic storms facing north-south facing to avoid maximum wind pressure on the windward side. Some villages are having high rise verandas on deposited mounds i.e. built on stilts to save structures from highly gusty wind. To have fewer traumas during storms the houses have puddled cladding as roof (Called ATTU) below the fragile thatched roof (Panda and Mishra.et al., 2020[15])

DRR on Cyclonic Storms

After the apaclyptic cyclone along Andhra coast in 1977, the cyclone review committee(CRC) has been formulated, under Science and technology Dept, GOI, and the cyclone mitigation plans such as Review of cyclone plan of India, zoning of cyclone prone areas and cyclone warning centres along coasts of India. There was need for preparation of national cyclone code, and CEAP's (cyclone emergency cyclone plans) in the coastal states in natinal level. There was need for cyclone research and training and accordingly the presentRSMC (regional specialised meteorological centres) and each state has its own national disaster response service givers (NDRF team) for authoritative retort to a menacing disaster state of affairs (Srinivas H N 2006[17]). Some indivisual DRR structures with 3D views are made on examplary basis which can withstand the disaster related hazards Fig 8 and Fig 9

DISCUSSION

About 75-80% of houses constructed today are non-engineered construction. For engineered construction the IS code 875 (Part-3) is used . For cyclone resielent structures, the points to be considered are choosing proper location, topography to avoid part of wind impact(Fig 9). The buildings should be of regular shape preferred circular or elecptical to evade concentrated pressure. Low height buildings are more preferable with roofing angle 22 to 45 degress to the ground with separate verenda or sitting place to avoid overhanging of wider roofs.The bonding between foundation wall and rof should be tight and bracings or more bands of concrete in the structure. Keep double doors and windows which should be firmly jointed to the structure. Avoiding light roofs like asbestos or tiles is a good decession. Plant trees at a distance to avoid wind pressure on the structure(Lakshman C T., 2011).

CONCLUSION

In moving towards a disaster resilient built environment, it is important that all the challenges discussed in the previous section are addressed effectively under the guidelines of Odisha State Disaster Agency (OSDMA) https://www.osdma.org/faq/reconstruction-of-school-buildings/ and Planning Commission, SER Division, GOI , New Delhi, guide lines. In addressing the challenges, participation of all relevant stakeholders, government or otherwise and the support of the community is highly appreciated. Investing in disaster resilient structure is better than investing to repair the structure after every calamity and keeping life in risk. Odisha has upheld its protest during emergency preparedness during Cyclonic storms..There were about 10,000 lives sacrificed during super cyclone 1999 Super Cyclone whereas the similar ESCS Fani (2019) has reduced it to 34 and close passing Amphan (2020) has zero mortality. It is high time for the to expedite to build and strengthen prevent cyclone resilient buildings and infrastructures to minimise trauma, deaths, devastations. Post-disaster construction should not be confined to only repairing the old one, They should be upgraded from pre-disaster levels.Temporary shelters should be built to higher standards so that later these can be used as housing for the poor or multipurpose shelters Maintenance funding for strengthening and retrofitting infrastructure could be increased by raising budget appropriations for this purpose.

REFERENCES

1. Chandra A, Williams M, Plough A, Stayton A, Wells KB, Horta M, et al. Getting actionable about community resilience: the Los Angeles County Community Disaster Resilience project. Am J Public Health. 2013 Jul;103(7):1181-9. PubMed PMID: 23678906. PMCID: Pmc3682620. Epub 2013/05/18. eng.
2. Jui-Sheng, ChouJia-Huei Wu, 2014, Success Factors of Enhanced Disaster Resilience in Urban Community, Natural Hazards,74(2):661-686; DOI: 10.1007/s11069-014-1206-4
3. Patel S. S., Rogers M. B, Amlôt R., Rubin G. J., 2017, What Do We Mean by 'Community Resilience'? A Systematic Literature Review of How It Is Defined in the Literature,http://currents.plos.org/disasters/index.html%3Fp=28783.html
4. Mishra S. P. and Panigrahi R. K., (2014), Storm impact on south Odisha coast, India, International Journal of advanced research in Science and Engineering , IJARSE, Vol. No 3,(11), pp 209-225
5. Li Z., Yu W ., Li K., Wang H., Liu Y., 2019, Environmental Conditions Modulating Tropical Cyclone Formation over the Bay of Bengal during the Pre-Monsoon Transition Period. Journal of Climate, 32(14), 4387-4394
6. Mishra Siba Prasad, Ojha, AnantaCharan, 2020, Analysis and Prediction of Upsurge in Cyclogenesis over the Arabian Sea Fabric, Journal of Xidian University, ISSN 1001-2400pp- 1275-1286Volume 14(5), 2020, https://doi.org/10.37896/jxu14.5/140
7. Code of Practice for Design Loads (Other than Earthquake) for Buildings and Structures - Part 3 : Wind Loads (IS 875 : Part 3) + Amendment 2016IS 875 (part -3) : the Bureau of Indian Standards
8. Bhandari N. M., Prem Krishna, KrishenKumar,Wind storms, damage and guidelines for Mitigative measures, IIT Roorkee, IITK-GSDMA-Wind 03-V3.0; 1-89, http://www.iitk.ac.in/nicee/IITK-GSDMA/W03.pdf
9. Gujarat State Disaster Management Authority, 2001, Guidelines for cyclone resistant construction of buildings in Gujarat, Gujarat, GSDMA, Gujarat State Disaster Management Authority, Government of Gujarat
10. Landsberg H. E, 1976, Weather, climate and human settlements, The World Meteorological Organization, special environmental report No.7, WMO aNo. 448 I, pp-13-15
11. Make the Right Connections; A manual on safe construction techniques prepared as part of the OAS/USAID Caribbean Disaster Mitigation Project (CDMP).
12. National Disaster Management Authority, Government of India, 2010, On Ensuring Disaster Resilient Construction of Buildings and Infrastructure financed through Banks and Other Lending Institutions

13. AgarwallAnkush, 2007, Cyclone resistant building architecture, Technical Officer (Hazard Vulnerability Reduction), GoI – UNDP, Disaster Risk management Programme
14. Gibbs T., 2001, Hurricanes and their effects on buildings and structures in the Caribbean, in: The USAID/OAS PGDM Building Inspector Training Workshop, Antigua, 2001.
15. Panda S., and Mishra S. P., 2020, Confronting and Coping with Resilient Environment by Fishermen Community of Penthakata, Puri during Fani, Adalya Journal, Volume 9, Issue 1, January 2020, pp- 230-242
16. Taher Rima, 2010, General Recommendations for Improved Building Practices in Earthquake and Hurricane Prone Areas, Prepared in the aftermath of the Haiti earthquake of 2010 for Architecture for Humanity, New Jersey Institute of Technology, College of Architecture & Design, University Heights,Newark, New Jersey 07102, USA, www.njit.edu
17. Srinvas H. N., 2006, Management of Natural Disasters in Developing Countries, proceedings of the Int. Workshop held in Asian institute of Technology (AIT), Bangkok, Thailand, 24-27; Daya Books, 2006 - Disaster management - 201 pages
18. C.T. Lakshmanan, 2011, Cyclone resistant structures, 2011. https://www.slideshare.net /ctlachu/43-final-cyclone-resistant-sturctures

Fig 1: A disaster risk resilent building in the villages of Coastal Odisha (Attu with Thatching)

Fig 2 : (A) Attu portion visible (b) Traditional informal storm resilient houses in tribal villages of Odisha

Fig 3: (A) Recently constructed cyclone shelter (B) Eroded post SuCS 1999 in JSPurOdisha, without care Source: https://www.thestatesman.com/cities/coastal-villages-jagatsinghpur

Fig 4: The heritagebuilding at Hukitola (1865) retained after combating many storms

Fig 5 :The roofblown away during ESCS Amphan in Kolkata 21st May 2020

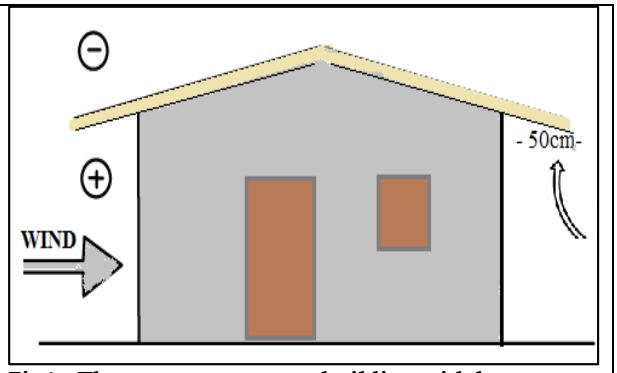

Fig6 : The pressure zone to a building with heavy wind (IS 875 (pt-3): 1987 revised 2015

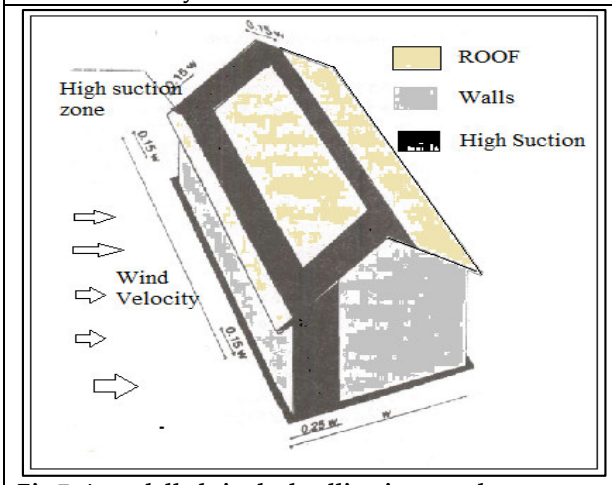

Fig 7: A modelled single dwelling in coastal are

Fig 8: Cover the pedestal by curtains to make it living but during storms stay at UG roo

Fig 9 : A mofel resilent building with large open spaces all around in the coastal areas

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RESEARCH ARTICLE

Comparative Haematological Studies of Both Male and Female Red Jungle Fowl (*Gallus gallus*)

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ABSTRACT

The present study based on analysis haematology of male and female Red Jungle fowls(*Gallus gallus*). The two different sex of fowl used as the experimental birds. This study had analysed the haematological profile of fowls male and female and the influence of sex on the haematological values. Blood samples were collected from both male and female fowls to study the following parameters Red Blood Cells (RBC), White Blood Cells (WBC), Packed Cell Volume(PCV), Haemoglobin (HB), MCV,MCH and MCHC . The mean value of haemoglobin (HB) concentration in males is 13.15±0.75 g/dl and 9.78±0.57 g/dl in females respectively. The mean value of RBC in males is $4.02\pm0.47\times10^{6}$ mm^3 and $3.64\pm0.36\times10^{6}$ mm^3 in females respectively. The mean value of WBC in males is $13681.0\pm713.425\times10^{3}$ mm^3 and 14198.2 ± 10^{3} mm^3 in females respectively. The mean value of PCV in males 49.27±0.86 % and 33.25±0.71 % in females respectively. The mean value of MCV in males 106.06±7.87 μm^3 and 91.98±7.19 μm^3 in females respectively. The mean value of MCH in males 32.35±1.46 pg and 26.98±1.45 pg in females respectively. The mean value of MCHC in males 30.57±1.18 % and 29.37±1.08 % in females respectively. The total red blood cells , haemoglobin concentration and packed cell volume of males red jungle fowl were higher than females ($p<0.05$). Finally MCV, MCH and MCHC of the male and female red jungle fowl were not significantly different ($p>0.05$).

Keywords: Haematological parameters, Red Jungle fowl(*Gallus gallus*), Haemoglobin, WBC, RBC

INTRODUCTION

Chicken is also referred as fowl which is descended from the red jungle fowl of Asia. When the first fleet arrived in Australia, the cargo includes poultry and since that time they have been many importance of poultry birds. The use of domesticated birds leads to the growth of a number of industries using various breeds to create products for human use (Carter and Howard,1923). The Red Jungle fowl (*Gallus gallus*) is a tropical bird in the family Phasianidae. It ranges across much of Southeast Asia and parts of south Asia. Red Jungle fowl are the primary progenitor of the modern chicken breeds used today in commercial agriculture (Daghir,1995). Red Jungle fowl has a mix of feather colours, with orange, brown, red, gold, grey, olive and metallic green plumage. The tail of the male roosters can grow up to 28 centimetre (11 inch) and the whole bird may be as long as 70 centimetre (28 inch). A moult in June changes the bird's plumage to an eclipse pattern, which lasts through October. There are 14 tail feathers. The male eclipse pattern includes a black feather in the middle of the back and small red orange plumes spread across the body. Female eclipse plumage is generally in distinguishable from the plumage at other seasons , but moulting schedule is same as that of males. The red jungle fowl body weight is around (2.5lbs (1kg) in females and (3.25 lbs (1.5kg) in males and brighten in colouration. This study was to establish the haematological values of the Red jungle fowl. From this study is important to assess the general health , clinical pathological diagnosis and in depth study of this bird.

MATERIAL AND METHODS

The mature Red Jungle fowls (Male and Female) was selected for this study, which was collected from this study, which was collected from nearly located poultry farm, Cuttack. The birds were obtained with their normal diet and environmental condition. The study was made on male(n=10) and female(n=10) Red Jungle fowl. Blood samples were collected from the wing vein of the fowls by the help of veterinary doctor. Blood samples were transferred in to 2ml EDTA vials for haematological analysis. All the samples were transferred in to the laboratory using icepacks within 12hr of blood collection. Haematological profile include total counts of RBCs, WBCs, Hb%, PCV which are estimated using the technique described (Cambell,2004). RBC, WBC counting was done by haemocytometer, the estimation of Hb% was carried out by haemometer and Packed Cell Volume measured using centrifuged machine.

RESULTS AND DISCUSSION

Haematology study of blood and blood related diseases and prevention of disease related to the blood. It involves treating disease that affect the production of blood and it's components, like blood cells, haemoglobin, blood vessels and the mechanism of coagulation. By studying these parameters of fowl helps in detection and diagnosis of diseases at an earlier stage. In this investigation haematological parameters like RBC, WBC, Hb, PCV, MCV, MCH, MCHC are analysed in both male and female fowl and comparison of haematological parameter between male and female is also presented. The mean haemoglobin concentration of Male Red Jungle fowl is 13.15 g/dl with a minimum range of 12.3 to maximum range of 14.2 g/dl and Female Red Jungle fowl have concentration of haemoglobin is 9.78 g/dl with a minimum range of 10.2 to maximum range of 12.1 g/dl.The Haemoglobin value differs from 13.15±0.75 and 9.78±0.57 g/dl respectively.The result shows that male fowl have comparatively high haemoglobin content as compared to female fowl. It may be due to direct effect of sex, hormones, both estrogens and androgens, on erythropoiesis. However since there is no difference in erythropoietin levels between the sexes . The result shows that male fowl have comparatively high haemoglobin content as compared to female fowl. It may be due to direct effect of sex, hormones, both estrogens and androgens, on erythropoiesis. Also the androgens have a stimulatory effect on EP secretion. Both these factors tend to keep the red blood cell count high in males which in turns causes high haemoglobin content and males are more prone to spikes of activity, while females do more sustained activity. So males evolved with a high level of haemoglobin to cover fluctuation (William et *al.*, 2010).

The total RBC values were not statistically different from each other. The TRBC values differs from 4.02 ± 0.47 to 3.64 ± 0.36 for Male and Female Red Jungle fowl respectively . The TRBC were higher in case of Male Red jungle fowl than the Female Red jungle fowl.Where as TRBC value of Male Red jungle fowl was tested by Jain et al.,(1993) which was slightly higher than the TRBC value of present experiment. However the result revealed that the TRBC value of two different sexes of fowl were not significantly different from each other. The result indicates that Total White Blood Cells (TWBCs) range from 13681.0± 713.42 to 14198.2 ± 726.40 for Male Red Jungle fowl and Female red Jungle fowl respectively . The TWBCs of Female red Jungle fowl was significantly higher than the TWBCs of Male red jungle fowl.The white blood cell has an important role in immunity system. When any bacteria , virus, fungi or any kind of foreign particles enters to body WBC can recognise it and protects body by fighting against it. As infection – causing bacteria or viruses multiply in the blood; bone marrow produces more white blood cells to fight off the infection (Dein FJ et al. , 1994).

The value of PCV for two different sexes ranges from 49.27 ± 0.86 % to 33.25 ± 0.71 % for Male Red Jungle fowl and Female Red Jungle fowl respectively . The PCV values were higher in Male Red Jungle fowl than the Female Red Jungle fowl. The difference was very large and was statistical different from each other. The PCV value of Male Red Jungle fowl was higher than the Female Red Jungle fowl. The haematocrit or PCV (Packed Cell Volume) have various relationship with the oxygen transport. The PCV value is optimum when the oxygen transport is more. The increasing value of PCV causes increasing the oxygen carrying capacity of blood as well as the exponential increase in bold viscosity (Birchard, 1997). The high PCV value causes an increasing of blood viscosity, which leads to reduce the blood flow and force the heart pump harder than the normal rate and to move the blood through the body (Clemens, 1990).

The MCV value for the two different sexes was ranges from 106.06 ± 7.87 to 91.98 ± 7.19 for Male and Female Red Jungle fowl respectively. MCV value was higher in Male Red jungle fowl than the Female Red jungle fowl. The result showed that the Mean Corpuscular Haemoglobin was varies from 32.35 ± 1.46 to 26.98 ± 1.45 for the Male and Female Red Jungle fowl respectively. The MCH value was higher in Male than the Female Red jungle fowl. For mean corpuscular haemoglobin concentration (MCHC) ,the MCHC value ranges from 30.57 ± 1.18 to 29.37 ± 1.08 for Male and Female Red Jungle fowl respectively. Values are expressed as mean ± standard deviation and significant at $p<0.001$, $p<0.01$ WBC= White Blood Cells, RBC= Red Blood Cells, Hb= Haemoglobin , PCV= Packed Cell Volume, MCV= Mean Cell Volume, MCH= Mean Corpuscular Haemoglobin, MCHC= Mean Cell Haemoglobin Concentration.

CONCLUSION

The result of this study provide the knowledge of the characteristics of haematological parameters of different sexes of fowls (*Gallus gallus*) differ from each other in various areas of world. In this study it was noted that the Red Jungle fowl of Haemoglobin , Packed Cell Volume, Mean Cell Volume, Mean Corpuscular Haemoglobin, Mean Cell Haemoglobin Concentration and Red Blood Cell is more in the male than the female fowl. In the WBC concentration is higher value in the female fowl than the male fowl.

REFFERENCES

1. Squires, E. J. and JULIAN, R. J. (2001). The effect of dietary chloride and bicarbonate on blood pH, haematological variables, pulmonary hypertension and ascites in broiler chickens. British Poultry Science, 42(2): 207 – 212
2. Mmereole, F.U.C. (2004). Hematological and Serological Profiles of the Local and Exotic Chickens in Southern Nigeria. PhD Thesis Submitted to the Department of Animal Science, Delta State University, Asaba, Delta State, Nigeria

3. Wikivet. (2012). *Chicken Haematology*. https://en.wikivet.net/chicken_haematol ogy. Accessed May 12, 2016. Buctot, FF &Espina, DM (2015). Breeding Performance and Egg Quality of Red Jungle Fowl (*Gallus gallus*L.) Under Confinement System .Journal Science, Engineering and Technology Vol. 4:65-75.
4. Christensen, K. D. (2014). Comparison of meta-analysis of the hematological parameters of commercial and indigenous poultry to wild birds: Implications to domestication and development of commercial breeds/lines. Journal of Veterinary Science and Animal Health, 1(1):1 – 12.
5. Arshad, M., M. Zakaria, A.S. Sajap and A. Ismail, 2000. Food and feeding habits of Red Jungle Fowl. Pak. J. Biol. Sci., 3: 1024-1026.
6. Ahlawat S. P. S., Senani S., Saha S. K., Rai R. B. Comparative production performance of Black Nicobari, White Nicobari, synthetic broiler and their crossbreds. Indian Journal of Animal Sciences 2001;71(11):1073–1074.
7. Aengwanich W and Tanomtong A (2007) Blood cell characteristics and haematological values of free ranging – red jungle fowl (*Gallus gallus*) in northeastern. Thailand Journal of Biological Science, 4: 689-692.

SL NO	HAEMATOLOGICAL PARAMETERS	UNIT	MALE (10)	RANGE	FEMALE(10)	RANGE	P Value
1	Hb	g/dl	13.15±0.75	12.3-14.2	9.78±0.57	10.2-12.1	0.082064
2	RBC	10^6/mm^3	4.02±0.47	3.16-4.80	3.64±0.36	3.13-4.23	0.050298
3	WBC	10^3/mm^3	13681.0±713.42	12480-14700	14198±726.40	13109-15100	0.068668
4	PCV	%	42.97±0.86	42.05-44.67	33.25±0.77	32.48-34.73	0.057332
5	MCV	Fl	106.06±7.87	91.77-113.95	91.98±7.19	82.10-104.50	0.000939
6	MCH	Pg	32.35±1.46	29.37-33.41	26.98±1.45	25.92-29.39	0.006481
7	MCHC	%	30.57±1.18	29.25-32.29	29.37±1.08	27.71-31.09	0.019723

Values are expressed as mean ± standard deviation and significant at $p<0.001$, $p<0.01$WBC= White Blood Cells, RBC= Red Blood Cells, Hb= Haemoglobin , PCV= Packed Cell Volume, MCV= Mean Cell Volume, MCH= Mean Corpuscular Haemoglobin, MCHC= Mean Cell Haemoglobin Concentration.

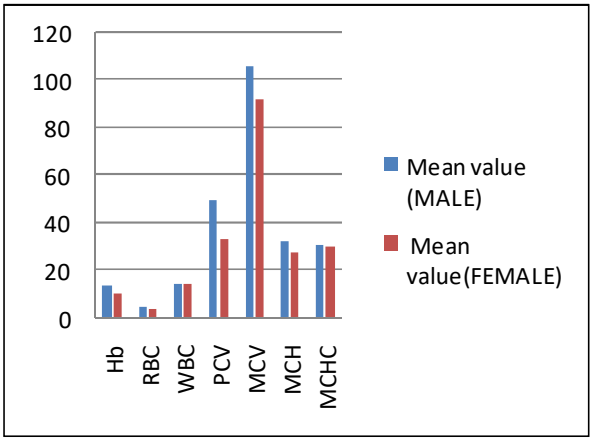

Fig.1. Comparative haematological values between male and female Red Jungle fowl

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RESEARCH ARTICLE

Problem of Malpractice in Private Engineering Institutions (Indian Context)

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ABSTRACT

In the last two decades the phenomenon of malpractice in examinations conducted by engineering colleges has seen a considerable rise. This enhanced the opening of several technical colleges mushrooming throughout the country .A new problem of large rise in enmass cheating has come up in many of the institutions .This has led to increase in large no.of unskilled engineers and their unemployment. Enforcement of all these steps with utmost sincerity and dedication will bring down malpractice in engineering institutions and the vast no. of unemployed engineers will also scale down

Keywords: phenomenon, Technical, colleges, engineers

INTRODUCTION

In the last two decades the phenomenon of malpractice in examinations conducted by engineering colleges has seen a considerable rise. It infact brings down the quality of the education imparted and employability in the market while tampering the image of technical education providing colleges in the nation (India). This paper throws light on this aspect and tries to counter it with some suggested measures

LITERATURE SURVEY

Economic reforms in 1991 by P.V Narasimha Rao Govt.(Prime Minister of India:1991-1996) guided by then Finance Minister Dr.Manmohan Singh aimed at rapid industrialisation ,foreign investment and encouragement to private sector along with the public by ending the licence raj. It led to increased investment and growth of private players in different sectors [1]. This enhanced the opening of several technical colleges mushrooming throughout the country. A new problem of large rise in enmass cheating has come up in many of the institutions .This has led to increase in

large no.of unskilled engineers and their unemployment [2] . Many business men, coaching centres owners and industrialists came up with engineering colleges owing to the increasing financial stability of middle class people thanks to nearly five decades of independence by 1990's .In the 1990's and early 2000's engineering education which was out of reach of many due to less no. of colleges became realizable for private colleges .As all the motive behind these educational institutions was business and profit, their evidently was lax in admission criteria's , procedures for allowing students who could just pay the desired fees .Many of these students had not worked sufficiently on Maths,Physics and Chemistry in their school and 10+2 exams .This weak mental ability and aptitude for sciences was accommodated to enrol in a professional and rigorous mathematical programme like Engineering.

Scenario in Private Technical Institutions

To increase the pass percentage the college management adopted certain manipulation techniques like:

1. Unfair use of technology (Xerox) or microxerox allowed into the exam halls with students
2. Backbiting and harassing the employment of lecturers and professors to loosen the vigil during examinations
3. Influential (close to the college proprietor) teaching and non-teaching staff involved in making answer sets to question papers for financial gain.
4. Hooliganism inside the college campus by students and previous year pass outs having backlogs
5. Backside financial gains for External supervisors from Universities for allowing malpractices during exams in back papers and special examinations.

Scenario in Europe

Malpractice in examinations is a universal phenomenon. It is linked to several social factors as well. The Pie chart below shows this problem by A.Bucciol, S.Cicognani and N. Montinari

Proposed Remedies

1. Minimum marks of 50% in 10+2 science and at least 60% in High school certificate examinations to restrict dull students getting admission
2. Students should be counselled in the first semester itself about examinations rules, regulations and consequences. They should be discouraged from copying.
2. Overall supervision of college admission, no. of students and their fees
3. Seizing of campus or blacklisting a certain exam hall on being caught copying
4. Supervision of video clips from CCTV footage of exam halls
5. Action on the charitable trust running the college (legal action) for not enforcing clean and proper examination procedures
6. Faculty recruitment procedure and removal to be supervised by a body of the university .The faculty should be paid at par with government scale of pay
7. Digital watches, cell phones and other audio visual equipments should not be allowed in the premises on the day of exam in line with national level examinations

CONCLUSION

Enforcement of all these steps with utmost sincerity and dedication will bring down malpractice in engineering institutions and the vast no. of unemployed engineers will also scale down.

REFERENCES

1. Ahluwalia S Montek "Indias Economic Reforms: Achievements and Next Steps"Review Article ,Asian Economic Policy Review /Vol.14,Issue 1

2. Engineering: "60% of engineering graduates unemployed" ,The Times of India Article 18th March 2017, www.timesofindia.indiatimes.com
3. Bucciol.A, Cicognani.S and Montinari.N,"Cheating in university exams: The relevance of social factors" Research Article Published (Jan.2020), International Review of Economics
4. 4.Samantha Subramanian "How cheating in India is a symptomatic of much bigger problem", Times of India article of March 20th, 2015
5. Sission .E, "Cheating in Engineering course :short and long term consequences ,1984
6. Srikanth.M, "Modern cheating techniques and their adverse effects on engineering"
7. "Indias cheating mafia gets to work", Article in www.the guardian.com
8. HE Campbell,Cheating ,Public administration education and online courses
9. HandingTreror, "Cheating in college and its influences on ethical behaviour in professional engineering practice" ,Kettering university
10. Hamzeh .D , "Undergraduate student cheating in exams" ,2012
11. Li Xiahong ,Meng Yaxin, "How to prevent college students fro cheating in exams?", IJRSEI2016,Vol.3,Issue 9
12. Bunn.DN, "An Economic analysis of undergraduate cheating behaviour"
13. Oliver Hartwitch, "The Economics of cheating" ,www. oliverhartwitch.com

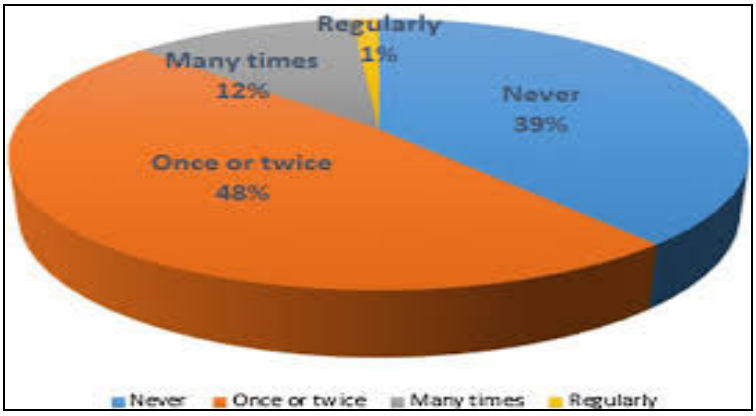

Fig.1: Cheating in University Exams[3]

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RESEARCH ARTICLE

Comparative Study on Haemato-Biochemical Profiles of Three Teleost *Labeo rohita, Mugil cephalus* and *Parastromateus niger* in Different Habitat

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ABSTRACT

Fishes are known as most useable protein source. Fishes are very sensible towards any environmental changes as they are familiar towards its surrounding. Haematological and Serum biochemical parameters act as the health indicator for fish as well as other organisms. In this study three fishes from different water such as; fresh water fish *Labeo rohita*, brackish water fish *Mugil cephalus* and marine water fish *Parastromateus niger* was taken in to consideration to assess the Haematological- biochemical analysis. The haematological analysis includes TRBC counting, TWBC counting, Haemoglobin percentage, PCV, MCV, MCH, MCHC and the biochemical analysis includes random plasma glucose, serum cholesterol, total protein and serum albumin. The TWBC value and PCV value was statistically significant at $P<0.001$. The TRBC value was significant at $P<0.005$.Whereas the Hb, MCV, MCH and MCHC value was statistically non-significant. On the other hand all the biochemical parameters of the above three fish species of different water such as; plasma glucose, serum cholesterol, total protein and serum albumin was statistically significant at $P<0.001$. The difference in all the haematological parameters between the three different fish species is due to change in ph and temperature of different water. The size of fish also affects the blood parameters of fish species. On the other hand all the biochemical parameters may differs due to feeding habit and any type of change in environment condition.

Keywords: Fish, Haematology, Biochemical, Marine, Brakish, fresh water.

INTRODUCTION

Fish is the notorious organism among the entire taxonomic group. It seems peculiar due its poikilothermic nature. Starting from its life, survival rate, appearance, reproduction ability and parental care, all these characters makes it different from others. During the period of evolution fishes shows most manifest feature. They can only survive inside water as they contain gills instead of lungs. From the ancient era and now a days also fishery acts as a foremost part of food source. It has been assessed that aquaculture i.e., mostly fish accomplishes the protein prerequisitearound 60% of people in India as well as several developing country (Osibonaet al., 2009). As fishery and its all-inclusive productshow this much of importance, thus it is very much crucial to taking care of fish health status and maintaining the breeding and development process of fish (Tripathi and Harsh, 2002).

Labeo rohita (F Hamilton, 1822) is the extensively used and easily available fish which is locally known as Rohu in India is a fresh water fish.Among cyprinids of all Indian major carp*Labeo*roita (Rohu) is the most preferable fish; hence it justify to be in the rank of a fish having higher economic importance.It mostly found in the rivers and backwaters of Northen India, Pakistan and Burma and also seen in the rivers of central region of India and Nepal(Chattopadhyay, 2017).*Mugil cephalus*(Linneaus, 1758) is a fish found in brackish water or marine water. It is also called as flathead grey mulletand it remains in the mouth of stream and river or in brackish bays, inlets and lagoons with sand and mud bottoms (Bester C, 2004).*Parastomateus niger* (Bloch, 1795) commonly known as and Black pomfret respectively are the well-known Indian marine fish and also found in western Pacific Ocean.

The physiological and haematological characteristics of a fish plays most vital role in knowing the health status of that species. The study of those characteristics of fish species is a considerable way get used in the progress of aquaculture. These tools may also help to know the good or bad health condition of an organism, if it is suffering from any type of disease or may facing any stress (RainzaPavia et al., 2000; O'Neal and Weirich, 2001).Any type of deviations in blood parameters may be seen due various factors such as; the fish species, aquatic biotope,age and sexual maturity,nourishment and health status of that species (Blaxhall, 1972; Chaudhuri et al. 1986; Wilhem et al. 1992; Hrubec et al., 2001; Fazio et al. 2016). Haematological parameters have an intimate relation with animal world and its health. It point out that haematological characteristics of a fish can be affected by the environment where the fish live i.e. any type of environmental disturbances can bring a immense change in the blood parameters of fish (Kori-Siakpere et al., 2005, Gabriel et al., 2004). This was conducted to determine the pathological condition of the three different fish species with respect to different type of water body such as; *Labeo rohita*, *Mugil cephalus* and *Parastromateus niger*.

MATERIALS AND METHODS

Experimental Site

This experiment was done from January to March 2020 at Centurion University of Technology and Management, Bhubaneswar, Odisha.

Experimental Species

The brakish water fishes *Mugilcephalus*(Linneaus, 1758) andmarine water fish *Parastomateusniger* (Bloch, 1795) was collected fromParadip, Jagatsinghpur, Odishafish market. Fresh water fish Labeorohita (F Hamilton, 1822) was collected from nearest fish market.

Data Collection

Blood samples were collected from the selected fish species (*Labeorohita*, *Mugilcephalus*and *Parastomateusniger*) for haematological and biochemical analysis. Blood samples were collected from the caudal vain of the above fishes by 2ml syringe (Dispo van, 26×1/2, 0.45×13mm, manufactured by: Hindustan syringe and medical devices Ltd., Ballabgarh,

Faridabad, India-121004) andinstantly placed in to an 2ml vials contained Ethylene diaminetetra acetic acid (EDTA anti-coagulant).Then the tube was thoroughly shake to mix the containing blood sample with the EDTA and then used for haematological analysis. Blood samples were marked according to types of species (2ml, XLNCA-E3K2,). For the biochemical analysis blood from the above specimen were collected and placed in to the appendorf tube.

Haematological Analysis

All the type of blood cell analysis was carried out including TRBC, TWBC counting, PCV, MCV, MCH, MCHC and MCHC calculation. The total Red blood cell and white blood cell count was done via haemocytometer. TWBC was done using Hayem's fluid and TRBC byTurk's fluid. Haemoglobin concentration was estimated by Sahli'shaemometer (Sahli's, 1909). The Packed Cell Volume (PCV) was measured by the help a windrop tubes placing them in a centrifuge machine at 3000 rpm for 5 min. Several erythrocyte indices like Mean Corpuscular Volume (MCV), Mean Corpuscular Haemoglobin (MCH) and Mean Corpuscular Haemoglobin Concentration (MCHC)was calculated by using respective formulas.

Biochemical Analysis

For the biochemical analysis blood was collected and segregation of serum from the blood sample was done instantly. The serum extraction was carried out by centrifugation of blood sample at 5000 rpm for 5 minutes. All the blood biochemical tests was conducted by using the standard methods and commercial kits (Coral Clinical System, Vernal Industrial Estate, Verna, Goa, India) such as; Plasma glucose estimation, serum cholesterol estimation, total protein estimation and serum albumin estimation.

Statistical Analysis

The results given in the study were obtained statistically analysis of the data. The haematological and serum biochemicalparameters were expressed as Mean±SE in all the three fish species i.e., *Labeo rohita, Mugil cephalul* and *Parastromateus niger* using the Microsoft Office EXcel 2010. Comparison of all the haematological and serum biochemical parameters in between *L. rohita*, *M. cephalus*and *P. niger*were performed in excel sheet by using ANOVA: Single Factor. Differences in between them were classified significant at $p<0.001$, $p<0.01$ and $p<0.05$

RESULT AND DISCUSSION

The haematological and Serum biochemical studies were equipped to compare all these values in between three fish species i.e., Labeorohita, Mugilcephalus and Parastromateusniger.

Haematological Analysis

Haematological analysis includes all the blood parameters such as; counting of WBC, RBC, percentage of Hb, PCV, MCV, MCH and MCHC (Table 1).

Total WBC Count

The TWBC values of three different fish species ranges from 8378.9±1045.611, 19044±2443.186 to 10624.1±388.6783 for *L. rohita, M. cephalus* and *P. niger* respectively. The obtained data indicates a statistically significant difference of TWBC value in between these three fish species at $P<0.001$ (Fig. 1) (Table 1). The TWBC value was higher in case *M. cephalus* and lower in case of *P. niger*. Varying in the WBC value indicates the variation in immunity system of different fish species of different waters. This value may vary with respect to different water(Mills and Fournier, 1979). WBC helps to indicate the diseased or non-diseased condition of a species. These changes may also indicate that marine water fish shows lower WBC value due to more pollution in marine water body.

Total RBC Count

The TWBC values ranges from 2.797±0.266254, 2.416±0.175722 to 1.767±0.135475 for *L. rohita, M. cephalus* and *P.niger* respectively.The result shows that the TRBC value for the three different fish species exist a statistically significant difference from each other at P<0.05 (Fig. 2) (Table 1). TRBC was more in *L.rohita* and less in *M. Cephalus* and *P. Niger* respectively.The TRBC value is related to haemoglobin concentration of that species. Higher RBC value implies that the oxygen carrying capacity was more in *L.rohita*i.e., more oxygen was needed for the body metabolism. Whereas a lower in RBC value indicates that *M. Cephalus* and *P. niger*can survive with a less consumption of oxygen (Acharya and Mohanty, 2014; Engel and Davis, 1964).

Estimation of Haemoglobin The haemoglobin percentage was ranges from 10.54±0.470744, 9.92±0.46111 to 8.88±0.58 for *L. rohita, M. cephalus and P.niger* respectively (Fig. 3) (Table 1). The Hb value of three different species was statistically non-significant. The Hb concentration was higher in *L. rohita*and lower in case of *M. cephalus and P.niger* respectively. The increasing or decreasing value of Hb is depends up the physical movement of a fish. The higher value of Hb in *L. rohita*indicates that it an active swimmer and more active than*M. Cephalus* and *P. niger*(Engel and Davis, 1964).

Estimation of Packed Cell Volume

A higher value of Packed Cell Volume was seen in case of *L. rohita*and for *M. cephalus* it was lower and lowest in *P. niger.* The PCV value for three different breeds of fish ranges from 28.1±0.982, 22.3±1.011599 to 20.9±1.206004 for *L. rohita, M. cephalus and P.niger* respectively. A statistically significant PCV value was exist for three different fish species at P<0.001 (Fig. 4) (Table 1). Varying in ranges of haematocrit or PCV value shows an inverse relationship with RBC. PCV and RBC value helps to know the anaemic condition of a species (Ahmadet al., 2015).

Estimation of Mean Corpuscular Volume

The MCV vale for three different fish species was statistically non-significant. The MCV value ranges from 114.2171±18.27246, 97.05369±8.653238 to 125.7603±13.52237 for *L. rohita, M. cephalus and P.niger* respectively (Fig. 5) (Table 1). The MCV value was higher in *P. niger*and lower in *L. rohita and M. Cephalus* respectively. The change in MCV value was due to fluctuation in the PCV and RBC values.

Estimation of Mean Corpuscular Haemoglobin

The MCH value for three fish species was ranges from 41.881±5.123, 44.4905±5.8707 to 52.334±4.349 for *L. rohita, M. cephalus and P.niger* respectively (Fig. 6) (Table 1). The MCH value was statistically non-significant. The MCh value was higher in *P. niger*and lower in *L. rohita, M. cephalus*. The change in MCH value was due to inclusive oxygen consumption rates and difference in swimming presentation under normal condition (Stillwell and Benfey, 1995).

Estimation of Mean Corpuscular Haemoglobin Concentration

A higher value MCHC was seen in *M. cephalu*and lower in *L. rohita*and *P. niger.* The MCHC value for three fish species was ranges from 38.1605±2.6233, 45.6151±3.3974 to 43.22002±3.0526 for *L. rohita, M. cephalus and P. niger* respectively (Fig. 7) (Table 1).The MCHC value was statistically non-significant. The varying ranges in MCHC of three different fish species may due to the increasing or decreasing values of Hb concentration and RBC values.

Biochemical Analysis

The biochemical analysis includes estimation of random plasma glucose, serum cholesterol, total protein and serum albumin.

Plasma Glucose Estimation

A high level of plasma glucose concentration wad found in *L. rohita*where the value was lower in *M. cephalus and P. niger* respectively. The plasma glucose concentration for the different fish species was ranges from 212.4±6.873,

62±1.498 to 56.7±1.826 for *L. rohita, M. cephalus and P. niger* respectively. The glucose concentration for three different fish was statistically significant at P<0.001 (Fig. 8) (Table 2). The higher level of glucose in *L. rohita* implies the stress condition. The variations in plasma glucose in different fish species with respect to different water is due to stress and fluctuation in fish species (McDonald and Milligan, 1992).

Serum Cholesterol Estimation

The cholesterol concentration for three fish was statistically significant at P<0.001 (Fig. 9) (Table 2). The glucose concentration ranges from 123.4±5.3483, 205.4±2.227 to 122.7±11.7142 for *L. rohita, M. cephalus and P. niger* respectively. The serum cholesterol concentration was higher in *M. cephalus*and was lower in *L. rohita*and *P. niger* respectively. The serum cholesterol concentration was different in different fish species due to deviation in their diet, their physical and sexual development as well as different activities (McDonald and Milligan, 1992).

Total Protein Estimation

The Total protein in blood was higher in case of *L. rohita*and lower in *M. cephalus and P. niger* respectively.Total protein value was ranges from 7.18±0.082, 5.44±0.089 to 4.61±0.12601 for *L. rohita, M. cephalus and P. niger* respectively (Fig. 10) (Table 2). The result shows statistically significance at P<0.001. Protein level of fishes acts as a display of nutritional value (Acharya and Mohanty, 2014). As *L. rohita*seems to contain higher value of protein it can be taken into consideration as a nutrient rich fish. Lowering the value of total protein than the normal range in blood plasma may indicate liver disease or a little infection. It also acts as a sign of immunodeficiency (Campbell et al., 2016).

Serum Albumin Estimation

The serum albumin concentration for three fish species ranges from 2.61±0.0721, 1.38±0.119 to 1.28±0.123 for *L. rohita, M. cephalus and P. niger* respectively. The serum albumin concentration was statistically significant at P<0.001 (Fig. 11) (Table 2). The serum albumin value was higher in *L. rohita*and lower in *M. cephalus and P. niger* respectively. Albumin is known to be the most profuse source of protein. It transport fatty acid to the liver and muscle cells for and later it used as an energy source. Hence, increase or decreasing value of serum albumin may be due to its extra synthesis or due to its loss through urine, faeces etc. Age, season,maturation, physiological status and geographical location of a fish also affects the albumin level of that fish. Fluctuations in the concentration of albumin of the above three different fish species such as; *L. rohita, M. cephalus and P. niger*from different water body may point toward that it was due to change in the environmental condition like fresh water, brackish water and marine water, ph level (Kovyrshina et al., 2012, Masi A et al., 2018).

CONCLUSION

Haematological and biochemical parameters can be known as a reflector of physiological and nutritional health.Aquaculture, ordinarily fisheries provides a huge amount of food and act as the largest protein source from the ancient period to the people and society. Management and protection of fish and a well organised fish culture influences the profitable use of fishes.In the above study three different fish species such as; fresh water fish i.e., *Labeo rohita*, brackish water fish i.e., *Mugil cephalus*, and marine water fish i.e., *Parastomateus niger* was takenand the haematological and serum biochemical analysis was concluded. Combining all the previous studies and this above study the conclusion says that fishes are very much serviceable and sensitive toward its natural environment. Now a day due to exposure of toxicants and heavy metals and several diseases caused by the nature leads fishes to stress condition, facing metabolic disorders, reproductive dysfunction and immunodeficiency (Filiciottoet al., 2012, Pradhanet al., 2012 and Handy RD, Depledge M H, 1999). Haematological and biochemical test was conducted to know the health status of fish and provide good health by knowing the diseases. The disturbances causes in the haematological parameters of fishes was due to less oxygen consumption, less active body metabolism of fishes, changes in environmental condition, stress, any type of destruction in gill. All the disturbances in serum biochemical parameters were due to change in ecological and biological characteristics of fishes as well as the changes in habitat of

fish. Diet also has a large impact up on the biochemical parameters, starving condition leads to fluctuation on amount of serum glucose level. At last, this study provides a brief data about the pathological condition fishes from different areas. Changes in several body parameters of fish in the evolutionary period due to environmental changes leads to lowering the economy as well. Studying up on these and monitoring the health status can helps to create awareness among the people to reduce pollution and protecting the fishes as a wild life as well as cultured organism to show the future generation.

REFFERENCES

1. RainzaPaiva MJT, Ishikawa CM, Das Eiras AA and Felizardo NN (2000)Haemotological analysis of 'chara' *Pseudoplatystomafasciatum* in captivity. Responsible aquaculture in the new millennium.Nice, France. European Aquaculture Society Special Publication; 28: 590.
2. Acharya G and Mohanty PK (2014) Comparative haematological and serum biochemical analysis of catfish *Clariasbatrachus*(Linnaeus, 1758) and *Heteropneustesfossilis*(Bloch, 1794) with respect to sex. Journal of Entomology and Zoology Studies; 2 (6): 191-197.
3. Ahmad Y, Andrabi SA, Hussain G, Wani AR, Bannetwala RC and Tharani M (2015) Haematological studies of fresh water fish, *Labeorohita* (Ham.) exposed to heavy metals. International Journal of Science, Environment and Technology; 4(6): 1513-1523.
4. Bester C (2004) Ichthyology at the Florida Museum of Natural History.
5. Blaxhall PC (1972) The haematological assessment of the health of the freshwater fish. A review of selected literature. Journal of Fish Biology; 4: 593-604.
6. Campbell CA, Georgiou A, Westbrook JI and Horvath AR (2016) What alert thresholds should be used to identify critical risk result: a systematic review of the evidence. Clinical chemistry; 62(11): 1445-1457.
7. Chattopadhyay NR (2017) Development of egg and spawn with special reference to Indian Major Carp.Induced Fish Breeding, 2: 15.
8. Chaudhuri SH, Pandit T, Banerjee S (1986) Size and sex related variations of some blood parameters of *Sarotherodonmossambica*. Environment and Ecology; 14: 61-63.
9. Engel DM and Davis EM (1964) Relationship between activity and blood composition in certain marine teleosts.Copeia; 3: 586-587.
10. Fazio F, Marafioti S, Sanfilippo M, Casella S and Piccione G (2016) Assessment of immune blood cells and serum protein levels in *Mugilcephalus* (Linnaeus, 1758), *Sparusaurata* (Linnaeus, 1758) and *Dicentrarchuslabrax* (Linnaeus, 1758) collected from the Thyrrenian sea coast (Italy). Cahiers De Biologie Marine;57:235–240.
11. Filiciotto F, Fazio F, Marafioti S, Buscaino G, Maccarrone V andFaggio C (2012) Assessment of hematological parameter range values using an automatic method in European sea bass (*Dicentrarcbuslabrax L.*). NaturaRerum; 1:29-36.
12. Gabriel UU, Ezeri GNO and OPabunmi OO (2004) Influence of sex, source, health status and acclimation on the haematology of *Clariasgariepinus*(Burch, 1822). African Journal of Biotechnology; 3: 463-467.
13. Handy RD, Depledge MH (1999) Physiological responses: their measurement and use as biomarkers in ecotoxicology. Ecotoxicology; 8: 329-349.
14. Hrubec TC, Smith SA and Robertson JL (2001) Age related in haematology and chemistry values of hybrid striped bass chrysops*Moronesaxatilis*. Veterinary Clinical Pathology; 30: 8-15.
15. Kori-Siakpere O, Ake JEG and Idoge E (2005) Haematological characteristics of the African snakehead, *Parachannaobscura*.African Journal of Biotechnology; 4(6): 527-537.
16. Kovyrshina, Tatyana B and Rudneva II (2012) Comparative study of serum albumin levels in round goby *Neogobiusmelanostomus*from Black Sea and Azov Sea. International Journal of Advanced Biological Research; 2: 203-208.
17. Masi A, Leboffe L, Polticelli F, Tonon F, Zennaro C, Caterino M, Stano P, Fischer S, Hägele M, Müller M, Kleger A, Papatheodorou P, Nocca G, Arcovito A, Gori A, Ruoppolo M, Barth H, Petrosillo N, Ascenzi P and Di Bella S

(2018) Human Serum Albumin Is an Essential Component of the Host Defense Mechanism Against Clostridium difficile Intoxication. The Journal of Infectious Diseases; 218 (9): 1424–1435.

18. McDonald DG and Milligan CL (1992) Chemical Properties of the Blood. In: W.S. Hoar, D.J. Randall and A.P. Farell (Edn). Fish Physiology of Academic Press Inc, San Deigo; 55-133.
19. Mills EL and Fournier RO (1979) Fish production and the marine ecosystem of the Scotian Shelf, Eastern Canada. Marine Biology; 54: 101-108.
20. O'Neal CC and Weirich CR (2001) Effects of low level salinity on production and haematological parameters of channel catfish (*Ictaluruspunctatus*) reared in multi-crop ponds.International Triennial Conference of World Aquaculture Society; 21-25.
21. Osibona AO, Kusemiju K and Akande GR (2009) Proximate composition and fatty acids profile of the African catfish, *Clariasgariepinus*. Journal of Life and Physical SCiencesActaSatech; 3: 85-89.
22. Patriche T, Patriche N and Tenciu M (2012) Cyprinids total blood proteins determination. Animal Science of Biotechnology; 42: 95-101.
23. Pradhan SC, Patra AK, Sarkar B and Pal A (2012) Seasonal changes in haematological parameters of *Catlacatla*(Hamilton, 1822). Comparative Clinical Pathology; 21: 1473-1487.
24. RainzaPaiva MJT, Ishikawa CW, Das EAA and Felizardo NN (2000) Haematological analysis of 'chara' *Pseudoplatystomafasciatum* in captivity. Responsible aquaculture in the new millennium. Nice, France. European Aquaculture Society Special Publication; 28: 590.
25. Sahli H (1909) Lehrbuchd.klin.Untersuchungen Method, Leipsic, 846.
26. Stillwell EJ and Benfey TJ (1995) Haemoglobin level, metabolic rate and swimming performance of triploid brook trout *Salvelinusfontinalis*. Journal of Aquatica; 137: 355-358.
27. TripathiG and Harsh S (2002) Fenvelerate-induced macromolecular changes in the catfish, *Clariasbatrachus*. Journal of Environmental Biology; 23:143-146.
28. Wilhem DF, Eble GJ, Kassner FX, Dafre AL and Ohira M (1992) Comparative haematology in marine fish. Comparative Biochemistry and Physiology; 102: 311-321.

Table 1 Haematological parameters of Labeo rohita, Mugil cephalus and Parastromateus niger

Sl. No.	Haematological Parameters	Unit	*Labeo rohita*	*Mugil cephalus*	*Parastromateus niger*	P Value
1	**WBC**	10^3/mm^3	8378.9±1045.611	19044±2443.186	10624.1±388.678	0.0001 S
2	**RBC**	10^6/mm^3	2.797±0.266	2.416±0.175	1.767±0.135	0.0041 S
3	**Haemoglobin**	gm/dl	10.54±0.470	9.92±0.461	8.88±0.5862	0.0843 NS
4	**PCV**	%	28.1±0.982	22.3±1.0115	20.9±1.206	0.00013 S
5	**MCV**	fl	114.2171±18.272	97.05369±8.653	125.7603±13.522	0.36109NS
6	**MCH**	pg	41.88188±5.1236	44.49051±5.870	52.334±4.349	0.34253NS
7	**MCHC**	%	38.16055±2.623	45.6151±3.397	43.220±3.052	0.22721NS

Table 2 serum biochemical parameters of Labeo rohita, Mugil cephalus and Parastromateus niger

Sl. No.	Biochemical Parameters	Unit	*Labeorohita*	*Mugil cephalus*	*Parastromateus niger*	P Value
1	**Glucose**	mg/dl	212.4±6.87378	62±1.49815	56.7±1.82605	2.22E-21 S
2	**Cholesterol**	mg/dl	123.4±5.34831	205.4±2.22711	122.7±11.7142	9.09E-09 S
3	**Protein**	g/dl	7.18±0.08273	5.44±0.08969	4.61±0.12601	5.97E-17 S
4	**Albumin**	g/dl	2.61±0.07219	1.38±0.11907	1.28±0.12365	1.45E-09 S
Figures in parentheses represent number of observation.Values expressed as mean ± standard error and significant at P<0.001, P<0.01 and P<0.05						

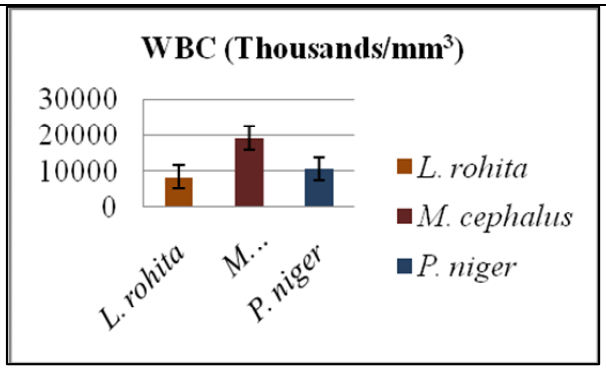

Fig.1 Comparison of WBC of *L. rohita, M.cephalus and Pniger.*

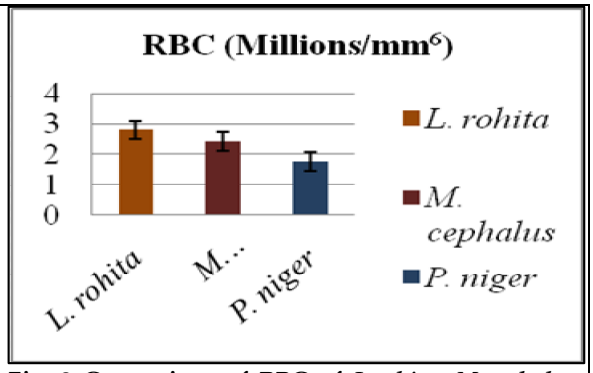

Fig. 2 Comparison of RBC of *L.rohita, M.cephalus and P.niger.*

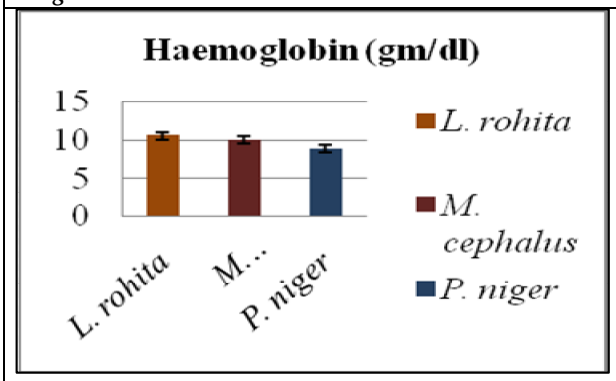

Fig. 3 Comparison of Haemoglobin of *L.rohita, M.lcephalus and P.niger.*

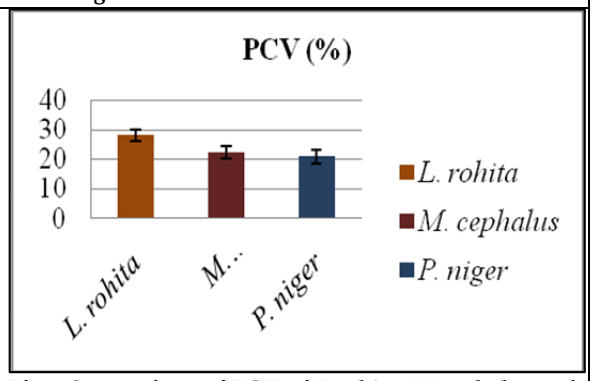

Fig.4 Comparison of PCV of *L.rohita, M.cephalus and P. niger.*

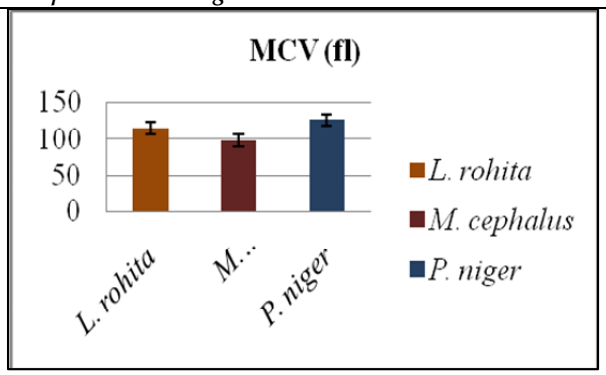

Fig.5 Comparison of MCV of *L rohita, M cephalus and P niger.*

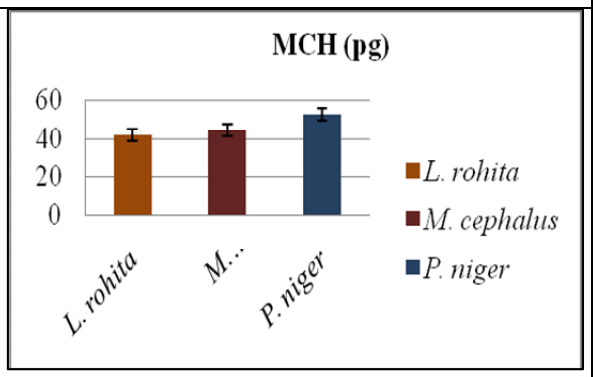

Fig.6 Comparison of MCH of *L rohita, M cephalus and P niger.*

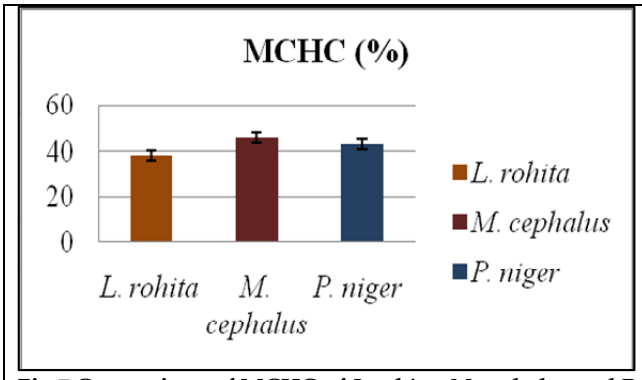

Fig.7 Comparison of MCHC of *L rohita, M cephalus and P niger.*

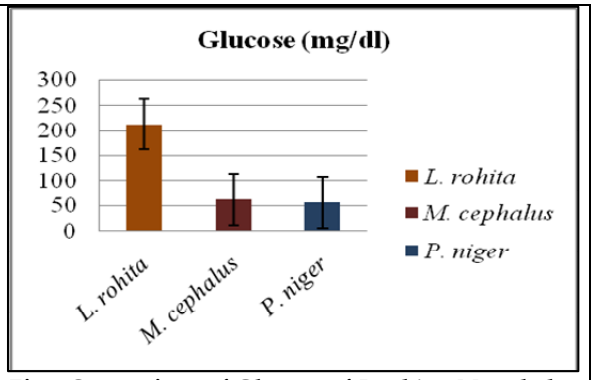

Fig.8 Comparison of Glucose of *L rohita, M cephalus and P niger.*

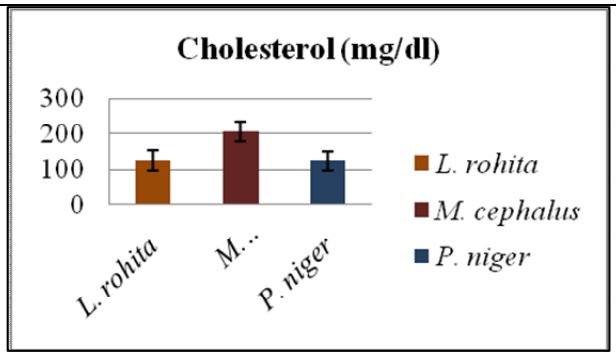

Fig.9 Comparison of Cholesterol of *L rohita, M cephalus and P niger.*

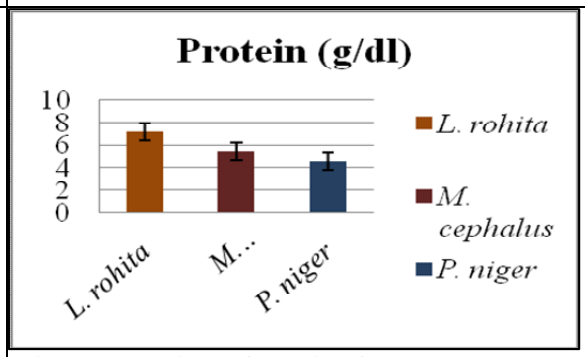

Fig.10 Comparison of Protein of *L rohita, M cephalus and P niger*

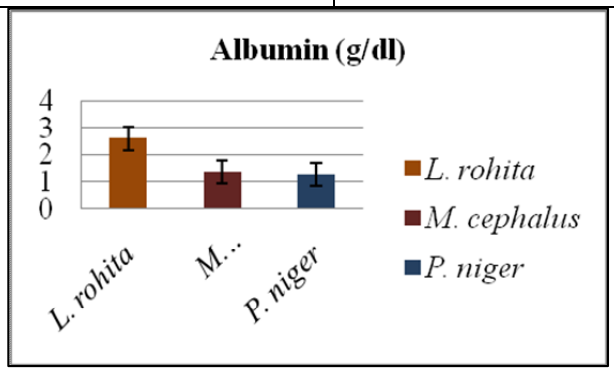

Fig.11 Comparison of Albumin of *L rohita, M cephalus and P niger.*

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RESEARCH ARTICLE

Effect of Malathion Exposure on Haematological Parameters of Fresh Water Fishes *Labeo rohita*

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ABSTRACT

Fishes are very sensitive to any changes in their aquatic ecosystem. Malathion is widely used as pesticide in agricultural field to protect the crops from pest. This pesticide causes significant changes in fish and may be fatal.In this study, the effect of malathion has been studied on haematological parameters of fishes.This present study concluded that significant variation in haematological profiles such as decrease in erythrocytes, haemoglobin, PCV, MCH,MCHC in fishes exposed to malathion than the control species labeo rohita without exposure.This studies sighted the effect of pesticides on fishes which will affect the biotic community and can provide the information to reduce the use of pesticide to maintain a safer and healthier environment for future generation.

Keywords: Malathion, Labeo rohita, haematological parameters

INTRODUCTION

Aquaculture is known as the largest sector for production of foods as it provides enough food sources. It is playing an important role in providing nutrition throughout the year. Fish provides a wide range of health benefits. Now uncontrolled use of pesticides in cultivated land and water bodies are the leading causes for pollution. Pesticides are the chemicals that kill the pest but having toxic effect on the environment. Pollution due to pesticides has a serious concern for the society. Globally, Pesticides are used to control the pest in agricultural field (Sarkar et al., 2004, Moore et al., 2011 and Vani et al., 2012). These pesticides come contact with aquatic ecosystem through different pathways. It ultimately affects the animal as well human health (Das and Mukherjee , 2003). Pesticides get used as a beneficial chemical agent by humans on the other hand it also affect the whole ecosystem and create disturbances in

the aquatic community (Gaafar et al.,2010). Among the organophosphate, malathion as pesticide causes harmful effect on vertebrates including mammals.Hence, the use of malathion is more frequent and regular than other pesticides (Pandey et al., 2005). It is highly toxic for aquatic biota (Areechon and Plumb,1990;Moore et al.,2011). Any type of contamination which may causes directly or indirectly occurs in aquatic body by pesticide may causes harm in fish production i.e.leads to decreases the amount of fish production (Jasmin et al.,2018). Blood parameter are very much sensitive to any changes in environmental factors that made easier to analyse (Remyla et al., 2008).

Haematological parameters are the well-known catalogues which have been chosen as the most important guide to identifying the health status, toxic effect and any damage in immune system of any living organism mostly the cultivated or domesticated animals (Thrall et al.,2012; Talas and Gulhan, 2009; Kavitha et al., 2010). Affected edible fish consumption may be affected the health of an individual. Fishes are very sensitive to water contamination by pesticide that can damage the different organs of fishes.Among the Indian major craps Labeo rohita (Hamilton,1822) commonly called as rohu is the most preferred species. It has certain advantages such as ability to thrive well in shallow waters, a high demand in market,excellent growth rate and it have the ability to survive in artificial diet also(Rani S et al.,2016). In recent years , haematology has been used as a tool to assess the physiological conditions in healthy, stressed or diseased fishes and also in toxicological screening culture of L. rohita and lack of information on haematology of this species (Rani et al,.2016). Hence, this study was find out the exposure of malathion on variation in haematological parameters of Labeo rohita.

MATERIALS AND METHODS

Study area

These investigation were was undertaken from the month of Decebe,2019 to Februay,2020. For this study fresh water fish species Labeo rohita were collected for the experimental work. The experimental analysis was done in the Zoology laboratory of Centurion University of Technology and Managemnt, Bhubaneswar campus, Odisha.

Collection of samples

The specimens were collected from the local market and ponds. These species were identified in the laboratory. Blood samples were collecte from the control fishes after identification of the species.After identification the blood samples were collected from the control species of L. rohita. Another one was kept under treatment with mallathione as pesticide.After sevendays, blood samples were taken for further analysis from both control and treated species.The collected blood samples were preserved in a 2 ml EDTA vials (Ethylene diamine tetraacetic acid)as anticoagulant agents for haematological experimental analysis (Parrino et al.,2018). These experimental analysis include Total Red blood cell count(RBC) using neubauer's chamber, concentration of haemoglobin (Hb) using Sahli'sHaemocytometer , White blood cell count (WBC) using Neubauer 's chamber ,packed cell volume (PCV) using wintrobe's tube, erythrocyte sedimentation rate(ESR) by Westergren method,Mean corpuscular volume(MCV), Mean corpuscular haemoglobin(MCH) and mean corpuscular haemoglobin concentration(MCHC) was determined by using standard procedure(Feldman et al., 2000). These were statisticallyanalysed and level of significance was considered at p-value<0.05. These data analysis of independent student t-test were carried out by Microsoft excel, 2010.

RESULT AND DISCUSSION

The reaction of fishes to many external factors is monitored by several changes in haematological parameters (Mazrouh et al.,2015). These parameters were stastically calculated and represented in table-1 as mean(X) ±SE of both two types of species with significant difference at independent t-test at p<0.05. During the study, one species was

kept under normal condition and another was treated with malathion. No mortaliry was observed during these seven days of control fish, but in treated fishes, behavioral changes were observed with redness of fins.

Estimation of WBC

The WBC value may use as the most important health indicator of a species. The WBC values ranges from 10694±540.709 to 6173.8±725.259 in control fish and fish affected with pesticide which implies that this value is statistically significant at $p<0.001$. A high value of WBC were observed in case of control fish i.e. Labeo rohita and lower in case of species with pesticides. The lower value of WBC in pesticide affected species may indicate that the species have less active immune system.Any change in environmental condition leads to change in the haematological parameters as they are sensitive to alterations in environment factors. These changes give clue to measure the illness or the disease of any species (Remyla S R et al., 2008).

Estimation of RBC

In case of control fishes, the value of RBC was higher than the fish affected with pesticide. The RBC was statistically significant value of both the species at $p<0.05$. The RBC value ranges from 2.416±0.191to 1.874±0.200 in control fish and fish treated with pesticide respectively.Some environmental factors like water salinity directly affect different parameters like RBC (Witeska 2013). The gathering of pesticide inside the gills of fish which was in pesticide control may show a decreasing level of RBC (Narain and Srivastava, 1989).

Estimation of haemoglobin

Haemoglobin concentration was different in case of both the species. The Hb value was more in case of normal fish than the fish affected with pesticide.These values ranges from 10.19±0.421492 to 5.12±0.235136, which statistically significant at $P<0.001$. The Hb value is very lower in case of the fish affected with pesticide this implies theoxygen consumption rate is very less. That leads to less iron flow through blood. The use of pesticides lowers the oxygen carrying capacity of body and may lead the fish towards death or diseased condition. The effect of the water salinity indirectly affects the oxygen carrying capacity of haemoglobin and thus the rate of oxygen transport may be increases or decreases (Witeska 2013) .

Estimation of PCV

The packed cell volume was ranges from 34.1±2.806 to 23.3±1.193 in control fish and fish treated with pesticide respectively. This value was statistically significant at $p<0.001$.A high level of PCV was noticed in control species where a very lower amount was found in case of the species with pesticide. The PCV value may decrease as the number of RBC reduces or their contraction in blood decreases (Singh and Srivastava, 2010). In general the decrease in RBC; successively moderate haemoglobin content and PCV value (Narainand Srivastava, 1989, Banaei et al., 2008).

Estimation of MCV,MCH and MCHC

The Mean Corpuscular Volume was varies from 158.42±29.64 to 139.31±16.79 which was statistically non-significant. The MCV value was higher in case of control species than the species affected with pesticide. MCH value was higher in control fishes as compare to the fishes with pesticides control. The MCH value ranges from 44.92±4.34 to 31.60±4.72. This value was statistical significant at $p<0.05$. The Value of Mean Corpuscular Haemoglobin Concentration (MCHC) was ranges from 31.60±2.49 to 31.60±2.49. This data shows the MCHC value was higher in case of fish with normal condition and lower incase of the species with pesticide control. The data is statistically significant at $p<0.01$.

CONCLUSION

This study will provide valuable information which might be helpful for fisheries and biologist in the assessment of fish health.Haematological indices are important for understanding the health status of an individual as well as status of animal population. Generally fishes are exposed to not only a single type of pollutant but also innumerable pollutants present in water bodies. The results from this earliest study provides the most uncomplicated and fundamental knowledge about blood cell contour of Labeorohita. This major carp has also both ecological and economic importance.From this study, it is also determined the effect of pesticide acts as toxicant for aquatic organisms and cause alternation in haematologicalincesand behavioural in this major carp. The presence of pesticides disturbs the aquatic ecosystem and fishes are not comfortable. Hence stringent care should be taken before using pesticide for environmental usage.

REFERENCES

1. Sarkar B, Chatterjee A,Mahapatra CT and Ayyappan S(2004).Effects of cypermethrin and carbofuran on certain hematological parameters and prediction their recovery in fresh water teleost,Labeorohita (HAmilton).Ecotoxicology and Environmental safe;58(2),220-226
2. Rani S,Nagesh TS ,Dash G and Abraham TJ (2016).Haematological.response of Labeo rohita (Hamilton) fingerlings exposed to low salinities. Indian journal of fisheries;63(2),127-131
3. Moore PD,Patlolla AK and Tchounwou PB(2011).Cytogenetic evaluation of malathion induced toxicity in Sprague-Dawley rats. Mutatio research/genetic toxicology and Environmental mutagenesis;752(1-2),78-82.
4. Vani T, Saharan N,Roy SD,Ranjan R,Pal AK,Siddaiah GM and Kumar R (2012).Alternation in haematological and biochemical parameters of Catla catla exposed to sub lethal concentrarion of cypermethrin.Fish Physiology and Biochemistry;38(6),1577-1584
5. Das BK and Mukherjee SC (2003).Toxicity of cypermethrin in Labeo rohita fingerlings:biochemical,enzymatic and haematological consequences.Comparative Biochemistry and Physiology Part C:toxicology and Pharmacology ;134(1),101-121
6. Gaafar AY,EI-Manakhly EM, Soliman MK, Soufy H,Zaki SM, Mohamed SG and Hasan SM (2010). Some Pathological, biochemical and haematological investigations on Nile tilapia(Oreochromis niloticus) following chronic exposure to edifenphos pesticide.Journal of American Science;6(10),542-551
7. Pandey S, Kumar R,Sharma S,Nagpure NS, Srivastava SK and Verma MS(2005). Acute toxicity bioassays of mercuric chloride and malathion on air breathing fish Channa punctatus(Bloch). Ecotoxicology and Environmental safe;61(1),114-120.
8. Areechon N and Plumb JA(1990). Sublethal effects of malathion on channel catfish,Ictalurus punctatus. Bulletin ofenvironmental contamination and toxicology;44(3),435-442.
9. Jasmin J, Rahman MM and Rahman MM (2018). Haematological changes in Labeo rohita (H.) due to exposure of pesticides Difenoconazole and Thiamethoxam.International Journal of Contemporary Research and Review; 9(01),20199-20205
10. Remyla SR, Ramesh M,Sajwan KS and Kumar KS(2008).Influence of zinc on cadmium induced haematological and biochemical responses in a fresh water teleost fish Catla catla.Fish physiology and Biochemistry;34(2),169-174.
11. Thrall MA,Weiser G,Allison R and Campbell T (2012). Veterinary haematology and clinical chemistry. John Wiley and Sons.
12. Talas ZS and Gulhan MF(2009). Effects of various propolis concentrations on biochemical and haematological parameters of rainbow trout(Oncorhynchus mykiss). Ecotoxicology and Environmental safe;72(7),1994-1998

13. Kavitha C,Malarvizhi A, Senthil Kumaran S and ramesh M(2010). Toxicological effects of arsenate exposure on haematological ,biochemical and liver transaminase activity in an Indian major carp,catla catla.Food and Chemical Toxicology ;48(10),2848-2854
14. Parrino V, Cappello T,Costa G,cannava C,Sanfilippo M,Fazio F and Fasulo S (2018).Comparative study of haematology of two teleost fish (Mugil cephalus and Carassius auratus) from different environments and feeding habbits. The European Zoological Journal,85(1),193-199.
15. Feldman BF,zinkl JG and Jain NC(2000).Schalm's Veterinary Hematology.5th edition,Lippincott Williams and Wilkins,1120-1124.
16. Mazrouh MM,Amin EM,Hegazi MA,Hussein KA and Attia ZI(2015). Some haematological parameters and blood picture of Oreochromis niloticus in Manzalah lake,Egypt.IOSR Journal of Environmental Science, Toxicology and Food technology;9(5),11-19.
17. Witeska M (2013) Erythrocytes in teleost fishes: A review Zoology and Ecology; 23(4),275–281.
18. Singh NN and Srivastava AK(2010).Haematological parameters as bioindicators of insecticide exposure in teleosts.Ecotoxicology;19(5),838-854.
19. Narain AS and Srivastava PN(1989). Anemia in the fresh water teleost,heteropneustes fossils under the stress of environmental condition. Bulletin of Environmental contamination and toxicology;43(4),627-634.
20. Banaei M,Mir VA,Rafei GR and Majazi AB(2008).Effect of sub-lethal diazinon concentration on blood plasma biochemistry.International Journal of Environmental Research;2,189-198.

Table 1 Comparison of haematological parameters of control species and pesticide affected species

Haematological parameters	Control species (Labeo rohita) (X±SE)	Specieswith pesticides (Labeo rohita) (X±SE)	p value
WBC (×103/mm3)	10694±540.709	6173.8±725.259	4.68E-05
RBC(×106/mm3)	2.416±0.191	1.874±0.2006	0.033
Hb (g/dl)	10.19±0.421	5.12±0.235	2.08E-09
PCV (%)	34.1±2.806	23.3±1.193	0.001
MCV (fl)	158.429±29.64	139.310±16.79	0.290
MCH (pg)	44.929±4.341	31.60235±4.728	0.026
MCHC (%)	31.602±2.497	22.587±1.677	0.003

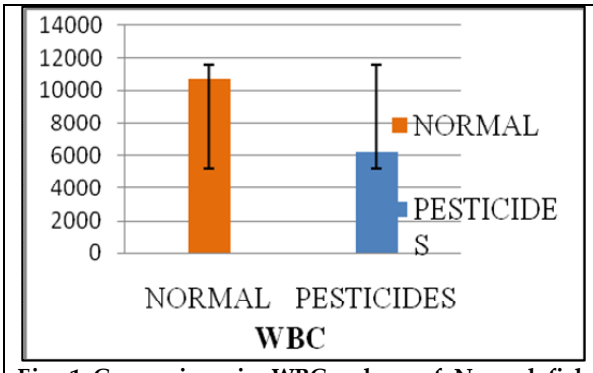

Fig. 1 Comparison in WBC values of Normal fish species and fish with pesticide control.

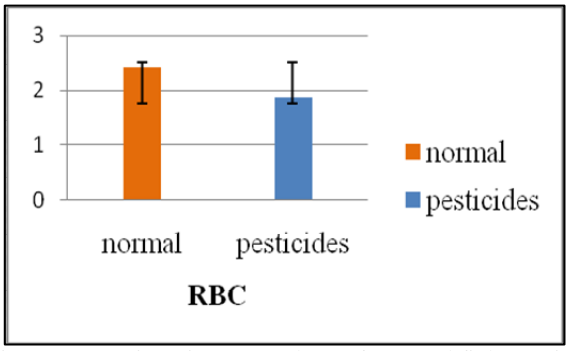

Fig. 2 Comparison in RBC values of Normal fish species and fish with pesticide control.

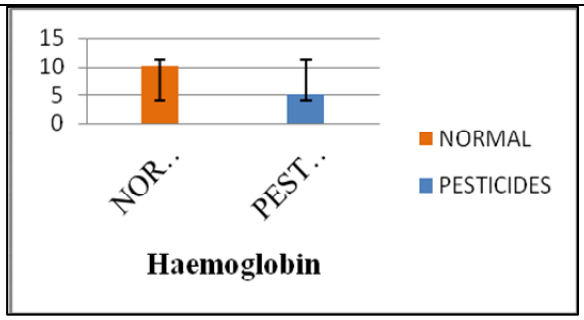

Fig. 3 Comparison in Haemoglobin values of control fish species and fish with pesticide .

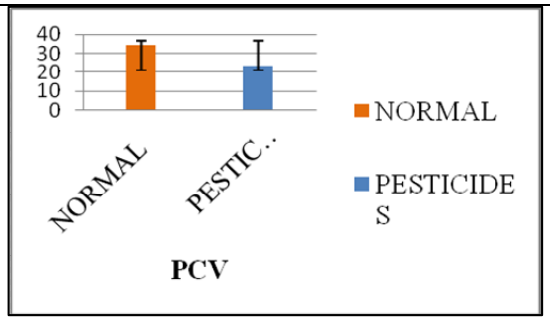

Fig. 4 Comparison in PCV values of Normal fish species and fish with pesticide control.

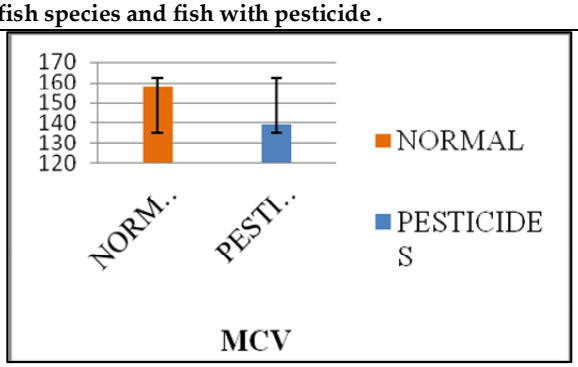

Fig. 5 Comparison in MCV values of Normal fish species and fish with pesticide control.

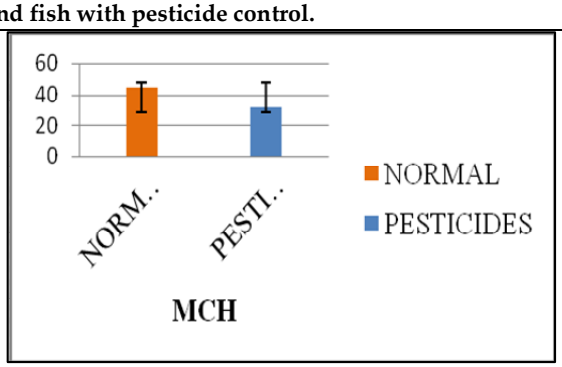

Fig. 6 Comparison in MCH values of Normal fish species and fish with pesticide control

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RESEARCH ARTICLE

Studies on Effects of environment on Haematological Profiles of *Mugil cephalus* (Linnaeus, 1758)

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ABSTRACT

Haematological parameters are found to be a useful implement for determining fish health. As *Mugil cephalus*(Linnaeus, 1758) belong to the omnivorous class and it can survive both brackish as well as fresh water environment.The main aim of this study was to find out the haematological parameters of *M.cephalus* which will provide a normal baseline values at a particular habitat. It can be used for comparative studies with other species and same species with other habitat.During this study following parameters were taken for haematological analysis such as total red blood cell count (RBC) and total white blood cells count (WBC), haemoglobin, mean cell haemoglobin concentration (MCHC), mean cell volume (MCV) and mean cell haemoglobin of *Mugil cephalus* . Haematological parameters were analysed by standard protocol The difference in all the haematological parameters between the fish species is due to change in salinity, pH and temperature of different water. The size of fish also affects the blood parameters of fish species. From this assessment, this study provides a better understanding of the influences of habitat and feeding habits on fish blood parameters.

Keywords: Haematology, *Mugil cephalus*, habitat, Fish health

INTRODUCTION

Fish cultivation is increasing to offset the shortage of animal protein worldwide. Mullets are distributed worldwide and live in tropical and temperate waters, and few spend their lives in fresh water as well [1]. It is found in coastal areas like lagoon and estuaries worldwide. In India, it is seen mainly in Kerala, Tamil Nadu, Andhra Pradesh and

Odisha. *Mugil cephalus* belongs to family mugilidae and includes 20 genera and 77 species in the world [2,3]. *Mugil cephalus* feeds mainly on zooplankton, benthic organisms and detritus. Local name and common name of *M. cephalus* are Khainga and Striped mullet respectively. It is the one of the most popular fish not only found in Chilika but also in worldwide because of its taste and commercial value. The species was very abundant in Chilika fishing decades ago, but is slowly becoming scarce due to various factors, such as overfishing, habitat loss, lack of breeding and nursery grounds, shocking migration routes to the sea, misuse of proper fishing networks and equipment etc.[4] Mugil cephalus not only occurs in the Chilika lagoon but also has a distribution worldwide where it inhabits estuarine, freshwater and marine coastal habitats. Despite such a large distribution and high commercial value, information concerning the growth parameters of this species for Chilika lagoon is very small. Base lines of haematological indices provide an important detector to know the physiological changes in the fishes. These parameters provide the information about the health status and toxicological symptoms of an organism.

It also shows adaptation capacity of that species to that specific environment [5]. Haematological parameters are considered to determine the status of a fish or fish population [6].These haematological parameters of fishes mainly depend upon the variation in sex, nutrition and environmental condition[7,8]. These variations are highly sensitive to environmental conditions like oxygen content, pH and salinity of water as well as the ecological factors[9]. Fish haematology helps us to find out the relationship with phylogeny,habitat and adaptation to specific environment[10].The haematological parameter are comparatively studied in different marine fishes. The result represents the haematological RBC, WBC , MCV and MCHC are significantly correlated[11]. The present paper focuses on profiling of haematological parameters of *Mugil cephalus* and will help in conservation of faunal diversity for sustainable management of Chilika lagoon.

MATERIALS AND METHODS

Study area

Chilika is the largest coastal lagoon in India and the largest brackish water lagoon in Asia. It is located(19°28′ to 19°54′N and 85°05′ to 85°38′E) in the Ganjam district of Odisha state on the East Coast of India. It is the largest coastal lagoon in India and the second largest brackish water lagoon in the world [12]. Analysis of haematological parameters and the experimental work was done in the Laboratory of Centurion University of Technology And Management, Bhubaneswar, Odisha.

Collection of sample

The specimens were collected from the fishermen and fish market of Chilika. The fish species was identified as *Mugil cephalus* by following the approach of Thomson (1984). Grey mullet (*Mugil cephalus;* Linnaeus 1758) were selected because of their year-round availability and high commercial importance. The blood sample was drawn from the caudal vein of fish by introducing disposable sterile 2.5 ml syringe. Then two ml of blood was transferred to anticoagulant vial containing EDTA (Ethylene-diamine tetra-acetic acid) for haematological analysis.

Haematological analysis

All the type of blood cell analysis was carried out including TRBC, TWBC counting, PCV, MCV, MCH, MCHC and MCHC calculation. The total Red blood cell and white blood cell count was done via haemocytometer. TWBC was done using Hayem's fluid and TRBC by Turk's fluid. Haemoglobin concentration was estimated by Sahli's haemometer. The blood was diluted with appropriate diluting fluid for RBC(Hayem's fluid) and WBC count(Turk's fluid) and were determined using Neubauer Chamber and observed under the microscope. The Packed Cell Volume (PCV) was measured by the help a windrop tubes placing them in a centrifuge machine at 3000 rpm for 5 min. Several erythrocyte indices like MCV,MCH and MCHC were indirectly by the above direct parameters values using standard formulas. Erythrocyte Sedimentation Rate (ESR) was estimated by the using Westergren pipette [13].These data were statistically analysed were carried out by Microsoft excel, 2010.

RESULT AND DISCUSSION

In haematological parameters of the *Mugil cephalus* (chilika Lake) were statistically analyzed and represented in Table-1.These tools or paprameters are essential tool for fish biologist and researchers in many parts of the world. These parameters are closely related to the response of the animal to the environment, an indication that the environment where fish lives could exert some influence on the blood characteristics (Fernandes and Mazon, 2003). Fish may be stressed when they are held and kept in captivity. Accordingly, the environment where the fish lives could exert some influence on the haematological characteristics of that species. However, the PCV values recorded in this study are 41±8.259%. Varying in ranges of haematocrit or PCV value shows an inverse relationship with RBC. PCV and RBC value helps to know the anaemic condition of a species [14].

Estimation of WBC

The total WBC count was varies from 11.286±1.953 $\times 10^3/mm^3$ in *Mugil cephalus*. The WBC value was higher in case of *M cephalus* which is either due to their feeding habitat of the species or environment since increased in salinity[15].

Estimation of RBC and Haemoglobin

A significant difference was found from the comparison between the total RBC counting at $P<0.01$. The TRBC value was ranges from $2.779\pm0.773\times10^6/mm^3$ in *Mugil cephalus*. Haemoglobin percentage in case of*Mugil cephalus* was mean±SD 10.35±0.732 g/dl. To remains more active a fish needed more oxygen which increases the Hb concentration [16]. RBC helps in transport of oxygen to the tissue and carbondioxide from the tissue to lungs. These variation in RBC could be due to the variation in ecological conditions[17].MCV is an estimate of the volume of RBC . In this study, it is determined that 41.246±16.986.However, the high MCV may be due to the high concentration of haemoglobin in red blood cells.

CONCLUSION

This preliminary study suggests that the disturbances in these blood indices were attributed to a defense reaction to stress due to the disturbances that occurred in fish exposed to acclimatization. In conclusion, this study has established influence of environment and habitat on haematological parameters in different habitat[18]. These results of haematological indices are considered as important tools for determining the health status of a fish by changing in adaptive physiological changes at a particular habitat. This investigation on fish haematology will provide a better contribution towards fish management. Such haematological findings from this study may represent the effective diagnostic tool for early understanding and the variability blood cells in different fish species.

REFERENCES

1. Nelson JS, Grande TC and Wilson MVH(2016) Fishes of the World. Fifth Edition, John Wiley and Sons, Inc., Hoboken, New Jersey.
2. Panda D, Mohanty S K, Pattnaik A K, Das S and Karna SK (2018) Growth, mortality and stock status of mullets (Mugilidae) in Chilika Lake, India. *Lakes & Reservoirs: Research and Management*, *23*(1), 4-16.
3. Turan C, Gürlek M, Ergüden D, Yağlıoğlu D and Öztürk B (2011). Systematic status of nine mullet species (Mugilidae) in the Mediterranean Sea. *Turkish journal of Fisheries and aquatic sciences*, *11*(2), 315-321.
4. Sahoo DK, Karna SK and Panda S(2012) Length Weight Relationship (LWR) and Growth Estimation of Mugil cephalus (Linnaeus, 1758) in the Chilika Lagoon, Orissa, India. Asian Journal of Experimental Biological Sciences,3(4),700-70.
5. Piccione G, Casella S, Lutri L, Vazzana I, Ferrantelli V and Caola G (2010) Reference values for some haematological, haematochemical, and electrophoretic parameters in the Girgentana goat. Turkish Journal of

Veterinary and Animal Sciences, 34(2):197-204.

6. Gabriel UU,Ezer GNO and Opabunmi OO(2004) Influence of sex,source,health status and acclimation on the haematology of *Clarias gariepinus*(Burch,1822).African Journal of Biotechnology,3(9):463-467.
7. Hrubec TC,Smith SA,Robertson JL(2001)Age related in haematology and chemistry values of hybrid stripped bass chrysops *Morone saxatilis. Veterinary Clinical Pathology,30(1):8-15.*
8. Fazio F, Marafioti S, Sanfilippo M, Casella S and Piccione G(2016) Assessment of immune blood cells and serum protein levels in Mugil cephalus (Linnaeus, 1758), Sparus aurata (Linnaeus, 1758) and Dicentrarchus labrax (Linnaeus, 1758) collected from the Thyrrenian sea coast (Italy). Cahiers De Biologie Marine,57(3):235-40.
9. Parrino V, Cappello T, Costa G, Cannavà C, Sanfilippo M, Fazio F and Fasulo S (2018) Comparative study of haematology of two teleost fish (*Mugil cephalus* and *Carassius auratus*) from different environments and feeding habits. The European Zoological Journal, 85(1):193-199.
10. Wilhelm Filho D, Eble GJ, Kassner G, Caprario FX, Dafré AL and Ohira M(1992) Comparative hematology in marine fish. Comparative Biochemistry and Physiology Part A: Physiology,102(2):311-321.
11. Satheeshkumar P, Ananthan G, Kumar DS and Jagadeesan L (2012) Haematology and biochemical parameters of different feeding behaviour of teleost fishes from Vellar estuary, India. Comparative Clinical Pathology,21(6):1187-1191.
12. Dujovny E (2009) The deepest cut: Political ecology in the dredging of a New Sea Mouth in Chilika Lake, Orissa, India. Conservation and Society, 7(3), 192–204.
13. Fernandes MN and Mazon AF (2003) Environmental Pollution and Fish Gill Morphology. In: Fish Adaptations, Val, A.L. and B.G. Kapoor (Eds.). Science Publication, Enfield, USA. 203-231.
14. Parvez F, Medina S, Santella RM, Islam T, Lauer FT, Alam N, Eunus M, Rahman M, Factor-Litvak P, Ahsan H and Graziano JH(2017) Arsenic exposures alter clinical indicators of anemia in a male population of smokers and non-smokers in Bangladesh. *Toxicology and applied pharmacology*, *331*, pp.62-68.
15. Maisano M , Natalotto A, Cappello T , Giannetto A, Oliva S, Parrino V , Sanfilippo M and Maucer A (2016). Influences of environmental variables on neurotransmission, oxidative system and hypoxia signaling on two clam species from a mediterranean coastal lagoon. Journal of Shellfish research, 35(1): 41-49.
16. Engel DM and Davis EM (1964) Relationship between activity and blood composition in certain marine teleosts. Copeia, 3: 586-587.
17. Orun I, Dorucu M and Yazlak H (2003) Haematological parameters of three cyprinid fish species from Karakaya Dam Lake, Turkey. *Online J. Biol. Sci*, *3*, 320-328.
18. Elahee KB and Bhagwant S (2007) Hematological and gill histopathological parameters of three tropical fish species from a polluted lagoon on the west coast of Mauritius. *Ecotoxicology and Environmental Safety*, *68*(3), 361-371.

Table-1 haematologival parameters of *Mugil cephalus*(Linnaeus, 1758)

Haematological parameters (Units)	Minimum value	Maximum value	*Mugil cephalus* Mean±SD(n=10)
Red blood cell ($\times 10^6$/mm^3)	1.18	3.95	2.779±0.773
White blood cell ($\times 10^3$/mm^3)	8.56	15	11.286±1.953
Haemoglobin (g/dl)	9	11.4	10.35±0.732
Pack cell volume (%)	28	52	41±8.259
Mean cell volume(fl)	108.1	303.5	158.979±62.88
MCH (pg)	26.7	83.05	41.246±16.982
MCHC (%)	17.3	38.62	26.475±7.129

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RESEARCH ARTICLE

Spatio-temporal Assessment of Butterfly Diversity Index in Some Areas of Puri, India

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ABSTRACT

A Study was undertaken to assess the butterfly area of "Deuli Matha", Kakatpur, puri (Latitude 19.9898* N; Longitude 86.1969*E). This place is adjacent to historical site of Mangala mandir temple, kakatpur expanding up to 1 to 2km, has enormous number of organisms and show a great area specifically in phylum Arthropods and class Insecta. Study was done to assess the butterfly area of this man-made garden from November 2019 to March, 2020 during morning 7.00am-10.00am and afternoon 3.30pm-5.30pm. As per the available data till date it was observed that, this beautiful place has 22 number of species belongs to order Lepidoptera under family Nymphalidae with eight species, Hesperiidae with three species, Pieridae seven species, Papillionidae three species and Lycaenidae one species. To assess the area statistically Simpson's diversity index was done. As an indicator this will help us to develop the environmental conditions of that area in a productive manner by taking necessary safety measures.

Keywords: Butterfly diversity, Diversity index, Insecta Indicator

INTRODUCTION

Insects are one of the most dominating creatures on the earth . Their population extended from frozen regions to temperate zone. It's been 200 million years they are being sustaining with more diversified way and plays a major role for maintaining the biodiversity and ecosystem. Diversity is the variability of living organisms including structural and genetic differences among group of individuals and between species. This concept of diversity is the major key factor for maintaining a healthy ecosystem. The world diversity is being maintained by 1,263,500 species of plants and animals while India is being a healthy resident for 51,828 species. Insects represent 80% of the total

species of kingdom Animalia throughout the world and according to the estimated data, there are about 9,50,000 species of insects and there so many yet to be discovered. Worldwide there are lots of organisms distributed with much diversity and specifically insects represent the highest among all and butterflies have been documented since 18th century [1].

A member of Hexapoda (Class-Insecta) belongs to the largest phylum Arthropoda. Characteristics of Arthropoda are little bit different from Insecta i.e.in terms of body segmentation. 1)Head contain mouth, compound eyes, antennae and antennules 2) Thorax divided in to 3 regions containing legs and wings 3) Abdomen contain all the organs such as digestive, excretory and reproductive[2]. One of the most identifying characters of insect is the presence of 3 pairs of legs. To identify such a higher group of organism classification is very much necessary. All insects belong to class insecta are grouped in two groups, such as Apterygota (wingless insects) and Pterygota (winged insects). Subclass pterygote is divided in to two divisions such as exopterygota and Endopterygota. Endopterygota further classified into 11 orders. Out of which Lepidoptera is one of them includes butterflies and moth has been evolved 35 million years ago and regarded as the major component of Biodiversity (New, 1991). Lepidopteran includes 1,50,000 species of butterflies, moths, and skippers[3]. Because of the body color and flying activities, these animals belong to order coleoptera. Butterflies are more familiar than night flying and dull colored moths. In terms of abundance and density, moths are more rather than butterfly, with certain exception.

Lepidoptera are widespread throughout the world except Antarctica. They are numerous and more diversified extends up to every corner of the world, from polar vegetation to desert and from mountain top to tropical rain forest. Butterflies get easily adapted to their environment according to their ecological niches but only shows restrictions when it comes to choosing host plants or nectar collecting plants. Abundance of butterflies at specific regions is due to availability of host plants and other resources. Sometimes it may cause problem because of insects which are injurious to human, agriculture, forest etc. because most of the injurious insects belongs to Lepidoptera. Lepidoptera divided into further families, such as Papilionoidae, Nymphalidae, Pieridae, Lycaenidae, Riodinidae, Hesperiidae. Butterfly has been one of the most efficient multitasking insects, act as pollinator, indicator of healthy environment, maintenance of food chain, supports other predator and parasite, shows mimicry, maintains biodiversity, population dynamics, natural pest controller etc. Butterflies have short life cycles and thus react quickly to environmental changes. Their limited dispersal ability, larval food plant specialization and close-reliance on the weather and climate make many butterfly species sensitive to fine-scale changes. Not all butterflies are flower visiting. Only those who have proboscis for feeding and liquid diet they pay visit to different flowering plants [4]. Because insects make up the largest proportion of terrestrial wildlife, it is crucial that we assess the fate of insect groups in order to monitor the overall state of biodiversity. Being typical insects, the responses seen in butterflies are more likely to reflect changes amongst other insect groups, and thus the majority of biodiversity, then established indicators such as those based on birds. The “Butterfly Effect”, a phenomenon in chaos theory is often used to explain the inherent complexity of weather system, researchers at the city based on Environmental Management and Policy Research Institute (EMPRI) Says that butterflies are the best bio-indicators of climate change. Asper the recent available data’s, butterflies have declined more rapidly than birds, plants and other organism emphasizing their potential role as indicators.

Butterflies are the most familiar insects to human being because of their bright color. Butterflies and moths are the only group of insects which have scales on their wings. There are about 17,500 species of butterflies present all over the world and around 750 butterfly species available at United States. They differ from other insects also by their ability to coil up their proboscis. So far 1,504 species of butterflies were recorded in Indian subcontinent [5,6,7] reported 334 butterfly species from the Western Ghats. In North-Eastern Himalayas, Evens (1932) found about 835 species, recently some new species were described and some extinct species were rediscovered, however these studies are mostly circumscribed to certain pockets.

Development of butterfly follows different stages to complete its life cycle, such as egg, larva, pupa and adult. Caterpillars are the larval stages of Lepidoptera have distinctive characteristics in terms of morphological feature which can be easily identified than the adults. While developing, their skin shed off four and five times called molting controlled by juvenile and Ecdysome hormones secreted from corpora allata and prothorasic gland respectively. With each molt, the coloration and appearance of the caterpillar changes leading to some changes. Relationship between host and depending animal is a real key factor behind existence of any organism, which provides the resources the development and growth. But as per certain data sometimes butterfly richness indicates low plant diversity but the exact region is still unknown [8,9].The aim of the study is to produce a report on available butterflies. to check the species richness and to study the interaction between butterflies and their respective host plants at study area.

MATERIALS AND METHODS

Study Area

The "Deuli Matha" is a very popular holy place of Kakatpur. Deuli Matha is situated near kakatpur, it is a holy place on the river bank of Prachi 1 km from Maa Mangala Temple, Kakatpur. 'Nabakalebara' of lord "Jagannath" the devotee prays the goddess "Maa Mangala" first & Maa direct them to go for Daru. The place is situated in the bank of river 'Prachi'. This place is 2 km far from Bajpur. It is known that this matha which is under the control of "Emar Matha", Puri is directly involved with Nabakalebara rituals of the Deities. The Even this matha is small but it has got an ancient status and tradition. A canal is flowing beside Deuli Matha which provides better environment and good place for the butterfly in Odisha.

Methodology

Observation was conducted from November 2019 to March 2020. It was done during morning 7.00- 10.00 am and evening 3.30pm to 5.30pm in these study areas. All the observation has been done by randomly just by walking at different parts of study area, mostly at flowering regions. Study was done by direct visual method. Cameras used were Samsung 6.0 mega pixels with 3X optical zoom and digital control. Flash was kept almost on to identify butterflies more efficiently. No animal was harmed during the study and it was carried out with lots of care and sincerity. Animals were identified by following data available on Indian Foundation for Butterflies (IFB)[10]. Based on the frequency of sighting, butterflies are divided in to three categories, such as Common, Uncommon and Rare.

RESULT

Diversity Indices

A diversity index is a quantitative calculation of species diversity in a community. It basically indicates the number of species i.e. Species richness as well as the abundance of each organism i.e. Evenness.

Simpson's index (D): It is actually a measurement of dominance.

$$D= \Sigma\, n(n-1)/N(N-1)$$

Where n is the total number of organisms of a particular species and N is the total number of organisms of all species.

Simpson's diversity index (1-D): The value of this index ranges between 0 and 1, so greater the value, greater the sample diversity. In this case, the index represents the probability that individuals randomly selected from a sample will belong to different species.

Table 1: Represents Simpson's diversity index

$D= \Sigma n (n-1)/N (N-1)$

$=328 / 83*82$

$=0.04$

Simpson's index (D) = 0.06

Simpson's index of diversity(1-D) = 0.94

DISCUSSION

During the study from November 2019 to March 2020, total 22 different species have been identified. All these species belong to 5 different families of Lepidopteran order. Out of 22 species, 8 species belong to family Nymphalidae, 3 species belong to family Papillionidae, 1 species belongs to family Lycaenidae, 3 species belong to family Hesperiidae, and lastly 7 species from family Pieridae. According to enlisted check list data, as per local status out of 22 species, 11 species belong to Common category, 2 species belong to uncommon category and 9 species belong to Rare category. Out of all the organisms most commonly available butterflies are Common evening Brown, Common branded Red eye, Common Emigrant, Monarch Butterfly, Red eyed, Evening brown Butterfly, Common Indian Crow, Indian Palm Bob, Common Crow, Danaid eggfly, Molted Emigrant found to be in maximum number around morning and afternoon time. Uncommon available butterflies Grey Pansy and Marius Hairstreak. Rarely available butterflies Peacock Pansy, Plain Tiger, Cabbage white, Crimson Rose, Large White, Blue jay, Indian Cabbage White, Shallow tails, Grass Yellow Butterfly. Species having abundant in number are called the dominant species, here the dominated ones belong to family Nymphalidae. There 8 different species of Nymphalidae has been found during the study period out of which Common Indian crow and Common evening brown are dominated ones. These are available at highest number.

Maintenance of healthy environment depends on living and nonliving factors and depending on the associative factors the number of organisms increases gradually. Communities can be large or small but each community consists of diverse species. All species are not equally important but everyone has some role in maintaining the richness. Species diversity is one of the most important and basic characteristics behind maintenance of a community as well as population. Higher diversity indicates better environmental conditions and other needed factors. There are various ways of measuring species diversity and it can be characterized by species richness and evenness of species abundance. By calculating all these aspects, we can get a better overview regarding the environment. Two most important aspects of biodiversity study are species richness [11] and relative abundance of individuals [12]. Here I have taken Simpson's diversity index to characterize the study area. These are commonly used parameters provide very much related data through which we can actual asses the study area as well as other outcomes. The data not only gives us idea regarding the available number of organism but also indicates the abundance of organism. To make sure I used the index called Simpson's diversity index, and the calculated value found to be 0.94. This index value lies between 0 to 1 which indicates that if the value is nearer to 1, then the area is more diverse or vice versa. As per the statistical analysis done above, the diversity indices such as Simpson's values showed higher diversity.

Nectar has all the nutritious materials that help for overall development of insects. Apart from this, through proboscis butterflies can draw nutrient from soil and mud because these things are rich in nutrients. But that is not enough for overall development, that's why caterpillars depend on leaves and butterflies depend on nectar containing flowers. Food is very much essential for overall development and for that the healthy physical property of soil is very much necessary. As we all know insects follow direct development shows different larval stage through metamorphosis for which hormones as very essential. At study area I got four different varieties of host plants, such as Dog wood, common Hoptree, Marigold and Leucanthemum species. These are all flowering plants produces nectars and that's why butterflies mostly rely on these plants for feeding and foraging. Any changes in physical properties of soil would ultimately affect the plants which will end up with affecting the respecting organisms who

depends on them completely. Since decades butterflies have been use as an indicator for the quantification of pollution and qualitative analysis of Environment [13]. Climate change has been one of the only reasons behind extinctions of lots endemic species in just two decades [14]. Change in Physical properties of soil or air or water is all because of human interference.

CONCLUSION

Environment is a home to all creatures of the universe, and the backbone of existence of life forms. So, there is no doubt in this that, this area is a very good resident for all its available organisms. Physical properties play an important role in determining soil suitability for agricultural, environmental and engineering uses. Availability of water and nutrient to plants its directly associated with physical properties of soil [15,16]. As this area is always been in a crowded condition because of human interferences so this is very prone to contaminations. Contamination leads to degradation of actual properties, so that control of human activities is very necessary. Habitat degradation, unsuitable resource exploitation, pollution, invasive species and climate change, the diversity of life on the planet is likely to continue life on the planet is likely to continue to diminish considerably over the coming years.

REFERENCES

1. Mohapatra R.K., Mishra A.K., Parida S.P. A Preliminary assessment of Butterfly diversity in Utkal University campus, Odisha. Zoo's Print, September 2013 Vol. XXVIII (9): pp 28-31.
2. Heppner JB(1998) Revised Family list for Lepidoptera. Lepidoptera news,3,57-59
3. Gilbert SF (2010). Developmental Biology. 9th Edition. Sinauer Associates, Inc. , Sunderland,USA.
4. Cranston P S and Gullan, PJ (2009) Phylogeny of insects. In *Encyclopedia of Insects* (pp. 780-793). Academic Press.
5. Wynter-Blyth MA (1957) Butterflies of the Indian Region. Bombay Natural History Society.
6. Smetacek P (1992). Record of Plebejus eversmanni (Staudinger) (Lepidoptera: Lycaenidae) from India. Journal of the Bombay Natural History Society89: 385-386
7. Gaonkar H (1996). *Butterflies of the Western Ghats, India including Sri Lanka: A biodiversity assessment of a threatened mountain system*. Centre for Ecological Sciences.
8. Larsen, N. (1986). *Quicksand; And, Passing*. Rutgers University Press.
9. Hawkins B A and Porter EE (2003) Does herbivore diversity depend on plant diversity? The case of California butterflies. *The American Naturalist*, *161*(1), 40-49.
10. Kremen C (1992) Assessing the indicator properties of species assemblages for natural areas monitoring. *Ecological applications*, *2*(2), 203-217.
11. Pathania PC, Mangat HK and Sidhu AK (2018). Studies on Butterfly Diversity (Lepidoptera: Papilionoidea) from Punjab Agricultural University Campus, Ludhiana, Punjab, India. *Records of the Zoological Survey of India*, *118*(1), 75-90.
12. Landau D, Prowell D and Carlton C E (1999) Intensive versus long-term sampling to assess lepidopteran diversity in a southern mixed mesophytic forest. *Annals of the Entomological Society of America*, *92*(3), 435-441.
13. Hamer KC, Hill JK, Benedick S, Mustaffa N, Sherratt TN, Maryati M and Chey VK (2003) Ecology of butterflies in natural and selectively logged forests of northern Borneo: the importance of habitat heterogeneity. Journal of Applied Ecology, 40, 150–162
14. Manzoor, M., Anwar, F., Sultana, B., & Mushtaq, M. (2013). Variation in antioxidant and antimicrobial activities in Lantana camara L. flowers in relation to extraction methods. *Acta Scientiarum Polonorum Technologia Alimentaria*, *12*(3), 283-294.
15. Pounds, J. A., Bustamante, M. R., Coloma, L. A., Consuegra, J. A., Fogden, M. P., Foster, P. N., La Marca E, Masters KL, Merino-Viteri A, Puschendorf R and Ron SR(2006). Widespread amphibian extinctions from epidemic disease driven by global warming. *Nature*, *439*(7073), 161-167.

16. Phogat V, Mallants D, Cox JW, Šimůnek J, Oliver DP, Pitt T and Petrie PR (2020) Impact of long-term recycled water irrigation on crop yield and soil chemical properties. *Agricultural Water Management*, *237*, 106-167.

Table 1: Representing list of butterflies found at study are Deuli Matha

Sl. No.	Common Name	Scientific Name	Family
1	Common Evening Brown	*Melanitis leda*	Nymphalidae
2	Peacock Pansy	*Junonia almana*	Nymphalidae
3	Monarch butterfly	*Danaus plexippus*	Nymphalidae
4	Common Branded Redeye	*Matapa aria*	Hesperiidae
5	Common Emigrant	*Catopsilia pomona*	Pieridae
6	Plain Tiger	*Danaus chrysippus*	Nymphalidae
7	Red Eyed	*Matapa aria*	Hesperiidae
8	Evening brown Butterfly	*Melanitis leda*	Nymphalidae
9	Cabbage White	*Pieris rapae*	Pieridae
10	Crimson rose	*Pachliopta hector*	Papillionidae
11	Common Indian Crow	*Euploea core*	Nymphalidae
12	Large white	*Pieris brassicae*	Pieridae
13	Blue Jay	*Graphium evemon*	Papillionidae
14	Indian Palm Bob	*Suastus gremius*	Hesperiidae
15	Indian Cabbage White	*Pieris canidia*	Pieridae
16	Grey Pansy	*Junonia atlites*	Nymphalidae
17	Common Crow	*Euploea core*	Nymphalidae
18	Danaid eggfly	*Hypolimnas misippus*	Nymphalidae
19	Shallow tails	*Papilio machaon*	Papillionidae
20	Grass Yellow Butterfly	*Eurema hecabe*	Pieridae
21	Marius Hairstreak	*Rekoa marius*	Lycaenidae
22	Molted Emigrant	*Catopsilia pyranthe pyranthe*	Pieridae

Table 2: Threatened List of butterflies found at the study area representing local status, WPA status and IUCN status

Sl. No	Common Name	Local Status	WPA Status	IUCN Status
1	Common Evening Brown	C		
2	Peacock Pansy	R		
3	Monarch butterfly	C		
4	Common Branded Redeye	C		
5	Common Emigrant	C		
6	Plain Tiger	R		
7	Red Eyed	C		
8	Evening brown Butterfly	C		
9	Cabbage White	R		
10	Crimson rose	R		
11	Common Indian Crow	C	Sch IV	LC
12	Large white(male)	R		
13	Blue Jay	R		
14	Indian Palm Bob	C		

15	Indian Cabbage White	R		
16	Grey Pansy	U		
17	Common Crow	C		
18	Danaid eggfly	C	Sch I	LC
19	Shallow tails	R		
20	Grass Yellow Butterfly	R		
21	Marius Hairstreak	U		
22	Molted Emigrant	C		

Table : 3

Sl. No	Common Name	Number of sample (n)	n-1	n(n-1)
1	Common Evening Brown	10	9	90
2	Peacock Pansy	2	1	2
3	Monarch butterfly	3	2	6
4	Common Branded Redeye	5	4	20
5	Common Emigrant	2	1	2
6	Plain Tiger	5	4	20
7	Red Eyed	4	3	12
8	Evening brown Butterfly	5	4	20
9	Cabbage White	5	4	20
10	Crimson rose	4	3	12
11	Common Indian Crow	5	4	20
12	Large white	5	4	20
13	Blue Jay	3	2	6
14	Indian Palm Bob	1	0	0
15	Indian Cabbage White	4	3	12
16	Grey Pansy	4	3	12
17	Common Crow	3	2	6
18	Danaid eggfly	7	6	42
19	Shallow tails	1	0	0
20	Grass Yellow Butterfly	3	2	6
21	Marius Hairstreak	1	0	0
22	Molted Emigrant	1	0	0
		Σ=83		328

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RESEARCH ARTICLE

Studies on Morphometric and Accumulation of Biometals in Fishes of Daya River near Bhubaneswar, Odisha

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ABSTRACT

The present study was carried out in Daya River near Dhauli, Bhubaneswar, Odisha to analyze the morphometric measurement and accumulation of biometals in some selected five different species. After analysis it was found that, there are 14 to15 different traced elements were accumulated in the tissues of fishes. Fourteen morphometric measurements were taken for the analysis of these five different fishes. The accumulations of biometals were studied by the X-Ray fluorescence spectroscopy. The study was found about 11 elements present in these species in ppm level. These biometals were determined the edible aquatic species like the *Puntius ticto, Amblypharyngodon mola, Cirrhinus reba, Penaeus monodon and Hypomesus olidus.* This investigation determined the accumulation of pollutant and trace elements in aquatic ecosystem and the aquatic adaptation of these species in these condition.It may help to monitor the quality of water that particular environment.

Keywords: Morphometric study, Biometals, Fish, Odisha, XRF spectroscopy

INTRODUCTION

The level of urbanization world over is on the rise as more than half (54.83%) are residing in the urban areas. Most of the world's major urban centres are nearer to the river basin. These river basin meet the requirements of urban areas world over like, domesic wastage, industrial activities and maintain the hydrological cycle. In India discharge of untreated sewerage is the leading cause of pollution of the rivers and other water bodies [1,2]. Bhubaneswar is one of the urban centres in the state of Odisha and Bhubaneswar as the capital of Odisha, which are situated along the banks of rivers Kuakhai and Daya. Bhubaneswar's population grew from 14512 in 1951 to 905339 in 2016 with

respect to the growing population of Odisha 44.86 billion. Generation of daily households and Industrial waste are being discharged into the rivers creating deterioration of aquatic environment. The municipal areas of Bhubaneswar is 135 Km^2 to 233 Km^2 and it lies between $20^012'$ N to $20^025'$N and Longitude $85^044'$N to $85^055'$N. The area used under residential, commercial, industrial, administrative, institutional and other utilities are 49.61 Km^2, 3.64 Km^2, 6.23 Km^2, 4.08 $Km^2$and 10.93 Km^2 respectively. Without treatment of effluent water, the waste water is discharged through Gangua nallah to the Daya River. Daya is a distributary of river Kuakhai which is a part of Mahanadi river basin. There are two industrial clusters consisting of 88 industries, 34 of which are vulnerable to water. Liquid waste in the form of domestic, biomedical and industrial waste has faced an acute disposal problem at the same time. The township is rapidly rising and all the liquid waste is drained directly to the Daya [3]. The fish has been treated as a staple food in around the world. Thus, in recent years there is an awareness of its nutritional and therapeutic benefit. Morphometric and meristic study of fish species is an important tool for accurate identification of the species using measurement of length , weight, fine count, spine count and other parameters [4,5].From some studies it is found that accumulations of biometals in various organs of fish may cause structural lesions and functional disturbances [6].According to Ahmad and Suhaimi-Othman (2010), the mature fish contain or accumulate more metals in their tissues as compared to the premature fish or old fish and that is due to the inhabitation of living continuously in that polluted environment or water.

MATERIALS AND METHODS

The fish samples are collected from the river and the fish market near Daya River. The collection of specimens and experimental analysis were done during the month of November,2019 to February,2020. During this study, five species including four fishes and one prawn were selected for this experimental approach. These collected specimens were *Puntius ticto, Amblypharyngodon mola, Cirrhinus reba, Hypomesus olidus* and *Penaeus monodon.* After collecting the specimens, these were preserved in10% formalin and stored in specimen bottle. Morphometric analysis was done of 14 parameters of fishes by using measuring scale and measured in centimetre (cm) in the laboratory of Zoology Department, Centurion University of Technology and Management, Odisha, India[8,9].

For analysis of biometals and trace elements in fish samples were analysed from the earlier samples preserved in bottle. One gram of accurately weighted dorsal tissues or muscles must be taken by dissecting for further analysis. Dissected samples were transferred to a Teflon beaker or petridish. Then the samples were placed in the oven for 2 to 3 days so that they can be easily converted into powdered form. Then the weighted samples were digested with 5ml of Nitric acid, then after complete digestion the samples were placed again in the oven for 15 mins at 180°C. Then the samples were cooled at room temperature and after that the samples were digested with 25ml of double distilled water. After adding double distilled water the mixture were stirred vigorously to get a samples solution for analysis of biometals by XRF spectrometer[10].

RESULTS AND DISCUSSION

The study on morphometric character in fishes is important because they can be used for the differentiation of taxonomic units and are able to spot from different fish population [11]. Morphometric analysis of these four different species has represented in table-1. General morphometric characters are influenced by various environmental factors. It has been reported that that hydro graphic condition may also led variation in body-proportion. So, the present study revealed that Morphometric analysis of freshwater fish of Daya river showed that the proportional growth rate of fish species increasing with increase in fish length and show the higher positive correlation with the total length. There may be some limitations which estimates that all measurements were obtained based on formaldehyde preserved specimens after 5-10 days of fixation. The change in the total length as well as total weight of the preserved specimen in formaldehyde is due to shrinkage and partial dehydration.The accumulation of biometals in particular species in particular amount is called bioaccumulation. A food chain is a

linear network of links in a food web. A food chain also shows how the organisms are related with each other by the food they eat. Due to eating some organisms of consumers that will accumulate more metals in secondary consumer, that process is called biomagnification. As a result, the elements present in consumer level that may get accumulated in the secondary consumer level and when we consume the secondary consumer the elements which get accumulated in his body from consumer level gets accumulated in our body. And as we consume fishes on the daily basis, the level of metals may rise up to the critical amount which may cause severe problems in human beings like it may damage the liver, pancreas, intestine, gall bladder, heart diseases, may secrete hormone higher than the normal amount[12,13,14].

In *Puntius ticto,* the traced metals are Ca>P>Si>S>K>Cl>Sn>Zn>Fe in which the required elements are Ca, P, Si, K, Cl, Fe. But Tin(Sn)which is not required element these may cause stomach ache, liver problem, kidney problem, tin leprosy etc. In *Amblypharyngodon mola, the traced metals are P>Ca>S>K>Cl>Sn>Fe>Eu* in which the required elements are P, Ca, S, K, Cl and Fe. But Tin(Sn) and Europium(Eu) is not the required elements. Although Europium is not an required elements but its advantages and disadvantages are not yet known.In *Cirrinus reba,* the traced metals are P>Ca>S>Cl>K>Sn>Fe>Eu in this the required elements are P, Ca, S, Cl, K, Fe. As we discussed before Tin (Sn) and Europium(Eu) is not the required elements.In *Penaeus monodon,* the traced metals are Si>K>Cl>Fe>Sn>Zn>Eu in this species the required elements are Si, K, Cl, Fe, Zn. In *Hypomesus olidus,* the traced elements are P>Ca>S>K>Cl>Sn>Eu>Fe in this the required elements are P, Ca, S, K, Cl and Fe. And as we discussed above Tin(Sn) and Europium(Eu) are the not required elements.

CONCLUSION

In conclusion, significant differences were identified among muscle of prawn and fishes, gill, liver, intestine of the fishes in view of the bioaccumulation of the selected heavy metals from Daya river. However, high level of heavy metals was found in liver and gill,but fish liver and gill are rarely consumed, it may represent good bio-monitor of metals present in the surrounding environment. So from the above discussion it is concluded that The Daya River is not that much polluted and the fishes came from that river are not much harmful for consumption. Bioaccumulation in living species can be reduced by proper management and treatment of waste material .

REFERENCES

1. Agrawal KK and Panda CR(2018)Assessment of water quality of river Daya at Bhubaneswar city, Odisha by using Water Quality Index Method, EM international, 37(1),117-126
2. Sridhar KS and Kumar S (2013) India's Urban Environment: Air/Water Pollution and Pollution Abatement. *Economic and Political Weekly*, 22-25.
3. Joshi A and Mishra SP(2017) Anthropocene effects on the river Daya and the lagoon Chilika by the effluents of Bhubaneswar city india: a physico-chemical study. International Journal of Advanced Research, *5(10), 1370-1384.*
4. Tacon AG and Metian M (2013) Fish matters: importance of aquatic foods in human nutrition and global food supply. *Reviews in fisheries Science*, *21*(1), 22-38.
5. Cavalcanti MJ, Monteiro LR and Lopes PR (1999) Landmark-based morphometric analysis in selected species of serranid fishes (Perciformes: Teleostei). *ZOOLOGICAL STUDIES-TAIPEI-*, *38*(3), 287-294.
6. Jezierska B and Witeska M (2006) The metal uptake and accumulation in fish living in polluted waters. In Soil and water pollution monitoring, protection and remediation (pp. 107-114). Springer, Dordrecht.
7. Ahmad A K and Shuhaimi-Othman M (2010) Heavy metal concentrations in sediments and fishes from Lake Chini, Pahang, Malaysia. *Journal of Biological Sciences,* 10(2), 93–100
8. Kamboj N and Kamboj V (2019). Morphometric and meristic study of four freshwater fish species of river Ganga. *The Indian Journal of Animal Sciences*, *89*(4), 470-473.

9. Talwar P K and Jhingran A G(1991) *Inland Fishes of India and Adjacent Countries*. Vol. 1 and 2. Oxford and IBH publishing house, New Delhi.
10. Swain S and Upadhyaya(2020)Elementary analysis of bhasmas used as ethnomedicine in tribal areas of mayurbhanj districts of Odisha, India. International Journal of Innovative Technology and Exploring Engineering,9(5),904-908.
11. Majumder A, Nanda BB, Naik AK, Misra SN (2019)Assessment of Quality of river water in the state of Odisha-A case study of the Rivers Kuakhai, Daya and Bramhani. International Journal of Innovative Technology and Exploring Engineering,8(7),83-87.
12. Jerome C and Pius A (2010) Evaluation of water quality index and its impact on the quality of life in an industrial area in Bangalore, South India. American Journal of Scientific and industrial research, 1(3):595-603.
13. Jayakumar P, Jothivel N, Thimmappa A and Paul V (2009) Physicochemical characterization of a lentic water body from Tamilnadu with special reference to its pollution status. The Ecoscan 3(1&2):59–64
14. Kar R and Swain S(2020) Influence of physico-chemical parameters on fish diversity in Paradeep coast, Odisha.Journal of Engineering sciences,11(4),1136-1138.

Table-1 Morphometric analysis of four different species

Sl No.	Parameters	*Puntius ticto*	*Amblypharyngodon mola*	*Cirrhinus reba*	*Hypomesus olidus*
1	Total length(cm)	7.5	8.1	21.5	11.8
2	Fork length(cm)	6.6	7.6	18.4	10.2
3	Dorsal fin(cm)	1.9	1.7	4.1	1.7
4	Pre-dorsal fin (cm)	3.3	3.5	7.1	6.6
5	Head length(cm)	1.5	1.9	3.1	2.2
6	Snout length(cm)	0.5	0.5	1	0.6
7	Eye diameter(cm)	0.5	0.4	1	0.6
8	Pre-pectoral fin(cm)	2.8	1.1	3.4	2.5
9	Pectoral fin(cm)	1.2	1.4	3.3	2.8
10	Pre-anal fin(cm)	4.4	4.7	14.1	6.9
11	Anal fin length(cm)	0.8	1.2	2.7	1
12	Caudal fin length(cm)	1.8	1.7	4.4	2.2
13	Pre-pelvic fin (cm)	2.9	3.6	7.7	5
14	Pelvic fin(cm)	1.4	1.2	3.3	1.5

Table 2: Element analysis by XRF spectrometer

	Puntius ticto	*Amblypharyngodon mola*	*Cirrhinus reba*	*Penaeus monodo*	*Hypomesus olidus*
Silicon	787.8ppm	192ppm	352ppm	478.9ppm	115ppm
Phosphorus	849.5	810.7ppm	655.4ppm	0ppm	784.6ppm
Potassium	267ppm	296.8ppm	148.6ppm	389.2ppm	278.9ppm
Calcium	993.1ppm	591.4ppm	393.6ppm	2703ppm	517.1ppm
Chlorine	190.1ppm	232ppm	212.6ppm	174.5ppm	193.3ppm
Manganese	0ppm	0ppm	0ppm	10.7ppm	0ppm
Iron	15.2ppm	16.9ppm	17.5ppm	66.2ppm	15.3ppm
Sulfur	432.7ppm	337.5ppm	280.2ppm	104ppm	378.7ppm
Tin	47.1ppm	71.9ppm	43.3ppm	48.6ppm	45ppm
Europium	21.7ppm	13.2ppm	4.1ppm	12.6ppm	20.2ppm
Zinc	0ppm	0ppm	0ppm	21.3ppm	0ppm

Fig1: Fishermen Fishing in Daya river, Odisha.

Fig2: collected five species for this study.

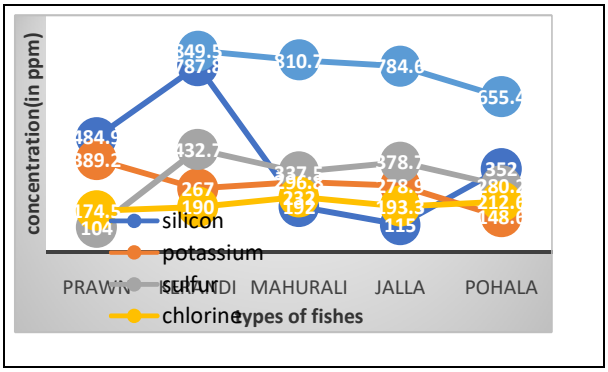

Fig.3 Comparative analysis of elements in selected species.

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RESEARCH ARTICLE

A Study on Assessment of Milk Protein of Some Indigenous Bovines of Odisha

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ABSTRACT

The present investigation was carried out to estimate the protein content, minerals and elements from different genotypes of dairy cows of Odisha. Protein estimation was done by following the general procedure of Lowry Method and XRF to determine the presence of elements in the milk sample of cow. These protein varieties contributes greatly to the unique nutritional and functional quality of milk obtained from different genotype of cows found in Odisha .A total of six dairy cows such as pure Indian breed desi cow(*Bos indicus*), Holstein, Gir , Hariana, Sindhi, Jersey were selected to conduct the experiment. From this experiment, it is showed that the protein from the given sample found to be more in desi cow milk (3.039) with 3.0366 ± 0.002074 µg/ml. The others sample from Holstein with2.17 ± 0.001581µg/ml, Gir with 1.995 ± 0.001581µg/ml, Hariana with 2.7452 ± 0.001924µg/ml, Sindhi with 2.7276 ± 0.00114µg/ml and Jersey with 2.427 ± 0.001581µg/ml. But the calcium, potassium and phosphorus is comparatively less in desi local cow milk and more in Jersey and Holstein breed. But chlorine and water content is found to be more in desi as compared to other breeds. From the above result it's been observed that the protein and chlorine is more with less thickness of milk lactation found in desi cow milk but other elements are more in other five breeds.

Keywords: Protein, elements, XRF, milk, cow.

INTRODUCTION

Milk is one of the highly evolve secretion of mammals by it provides the better nutrition to the infants(1). Milk from dairy meets the nutritional requirements as compared to any single food and is regarded as ideal and complete food(2). India is considered as the largest consumer and producer of milk in the world. There is a growing public

health issue in the recent past, especially according to our intake of food. Milk contains about 86% of water,4.6% lactose sugar, 3.7% triglycerides, 2.8% milk protein with 0.54% minerals(3). Milk is used for the preparation and production of various valuable nutritional items. The milk composition is influenced by sex, sex, lactation period, diet and environment. A number of authors have shown that variations in the chemical and physical chemical properties of milk are determined by genetically variation among cows of different races(4). In recent days, great attention is given to milk from indigenous cow and buffalo, as they produce A2 milk which is safer than A1 milk produced from exotic. Milk A1 contains A1β Casein and milk A2 contains Milk that contains A2β-Casein respectively. A1 milk protein generally found in European crossbreeds while indigenous cows and buffaloes contain A2 milk in India(5). The physico-chemical and nutritional values of cow's milk are more significant and its industrial production capability varies by many factors. These are including: diet, type of breeds, feeding and environmental condition.The price of cheese has risen in recent years and therefore the assessment of the protein content of milk is an important factor in the quality of the industry(6). In the near future, milk components, such as milk fat, particularly protein, will be more important when it comes to milk quality. It needs continuous monitoring of milk protein and simultaneous work on genetic development in this way. The object of the study was to investigate the assessment of protein in five different breeds of indigenous cows of Odisha.

METHODOLOGY

This experimental study was undertaken at the department of Zoology and ATC laboratory of Centurion University of Technology and Management, Bhubaneswar campus, Odisha from the month of November, 2019 to December,2020. This study was consisting of two parts. One part was considered for protein analysis by Lowry's method and another part included the analysis of trace elements present in the milk samples(7).

Preparation of Stock Solution

The day before the experiment the stock solution need to be prepared from the egg white. First of all egg albumin was collected by piercing a small hole using a sharp needle and then collected in a clean beaker measuring exactly around 10ml. Then 10ml distilled water added to it and stirred with the help of a stirrer. Then from the mixture another 10ml was taken in another clean beaker, where 50ml of distilled water was added. The mixture is kept inside laminar airflow chamber for the whole 24hours for it to settle down.

Collection of Milk Sample

All the milk samples were collected in well cleaned plastic bottles from the dairy farm of CUTM Campus except the Desi cow milk which is collected from the locality of Bhubaneswar. The milk was collected early morning before 8.00 a.m. soon after the milking of cows. Since the milk used to get spoil within 3 to 4 hours from the time it has been collected. Therefore the milk samples were storaged inside the deep freezer if not able to conduct the experiment within 3 to 4 hours of its collection.

Normalizing the Freezed Milk

Just before conduct the experiment, the freezing milk samples were normalized where the milk reaches to the normal temperature and ready for the experimental use. After normalization of different milk samples of different breeds, total protein present in milk samples were estimated according to Lowry's method by using UV visible spectrophotometer [6]. The following reagents were used during the protein analysis by Lowry's method. Folin ciocalteau reagent(Reagent D), The reagent should have no greenish 20%sodium carbonate in 0.1N sodium hydroxide (reagent A).Reagent B was prepared with 0.5% copper sulphate in 1%pottassium sodiumtartrate. Then Alkaline copper solution (Reagent C) was prepared by mixing of 50ml of reagent A and one ml of reagent before use. The day before experiment, stock solution need to be prepared by mixing of ten milliliter albumin added with 10 ml of distilled water. Standard solution was prepared by 10ml stock solution added with 50ml distilled water.The amount of protein present in milk was measured using a calibration curve prepared with different concentrations

albumin as standard. In a series of test tubes different aliquots of standard protein solution were pipetted out. For protein analysis, supernatant were collected after centrifugation. Centrifuge tubes were taken and Pipette out 0.2, 0.4, 0.6, 0.8 and 1.0ml of the working standard into a series of test tubes. All tubes were made up of volume up to one milliliter. Took six clean test tubes were taken where in the first tube only 1ml of distilled water is taken. In the 2nd tube 0.2ml of Stock solution with 0.8ml distilled water to make it total 1ml. then in the 3rd tube 0.4ml of Stock solution with 0.6ml of distilled water. In the 4th tube 0.6ml of Stock solution with 0.4ml of distilled water. In the 5th tube 0.8ml of Stock solution with 0.2ml of distilled water.

Then 5 ml of reagents were added to each test tube and mixed thoroughly. After ten minutes 0.5ml of reagent D was added in each tube. These tubes were mixed immediately after each steps of addition and placed at 37^0C for 30 minutes. Purple blue colour was developed and readings were taken in spectrophotometer at 640 nm. A standard graph was drawn to calculate the amount of protein present in respective sample in the sample.Optical Density is measured in the spectrophotometer at wavelength 640nm. Then serially all the test tube's components are measured keeping the manual setting as per the requirement. All the above procedures were done for 6 times as the experiment consisting milk samples of 6 genotypes of cow available in Odisha. For the analysing elements present in milk samples of different milk sample of Indian cows, the fresh milk were collected and analysed by XRF spectrophotometer in ATC laboratory of Centurion University of Technology and Management, Bhubaneswar campus, Odisha. The samples were tested and results were obtained for the experimental analysis.

RESULTS AND DISCUSSION

The study was under taken to find out the protein content in milk of different breeds of cows and simultaneously the trace elements present in the samples also analysed during the investigation. These breeds are generally domesticated in rural areas only for their lactating behaviour. Although the breeds are very good in lactating good amount of milk, but the protein content is more in Desi cow *Bos indicus* with 3.0366 ± 0.002074 µg/ml. The samples from other breeds have the milk content as follows like Holstein with2.17 ± 0.001581µg/ml, Gir with 1.995 ± 0.001581µg/ml, Hariana with 2.7452 ± 0.001924µg/ml, Sindhi with 2.7276 ± 0.00114µg/ml and Jersey with 2.427 ± 0.001581µg/ml. As the milk contains a wide range of minerals, some minerals were analysed during the study. Here these data were enlisted in table-2 after analysing by XRF spectrophotometer (8).Minerals like Calcium, potassium and phosphorous concentration were less in milk of desi cows as compared to the bovine species. But the water and chlorine content is more in milk of desi cows as compared to others breeds. The quantity of milk varies according to the genetics and inheritance of the lactacting character. The concentration of protein in milk is not directly associated with quantity of milk secreted from cow. Thus further study should be undertaken to enhance the protein values long with the production of milk.

CONCLUSION

Milk provides a significant amount of nutrients which is required for the development of human individual. As necessary elements it takes part in several metabolic pathways and regulates the positively effect on blood pressure and oxidation for maintaining good health(9). Protein from different breeds of dairies varies according to the climatic condition and other biological factors(10). For quantity and nutritional aspects selective breed can be domesticated. The protein content with their medicinal values with their selective breeds can improve the diary as well as pharmaceutical industry.

REFERENCES

1. Reddy PR, Reddy AN, Ramadevi A and Kumar DS(2016) Nutritional significance of indigenous cow milk with regard to A2 beta casein–An overview. International Journal of Science, Environment and Technology,5(5):3376-3380.
2. Veeresh HB, Poornachandra KT and Srinivas B (2019) Comparative Investigations of Milk Quality from Holstein Friesian Cross Breed and Indigenous Deoni Cows. International Journal of Agriculture Sciences, 11(11), 8612-8613.
3. Nickerson SC (1995) Milk production: Factors affecting milk composition. In *Milk quality* (pp. 3-24). Springer, Boston, MA.
4. Mishra BP, Mukesh M, Prakash B, Sodhi M, Kapila R, Kishore A, Kataria RR, Joshi BK, Bhasin V, Rasool TJ, Bujarbaruah KM(2009) Status of milk protein, β-casein variants among Indian milch animals. Indian Journal of Animal Sciences,79(7):722-725.
5. Sodhi M, Mukesh M, Kataria RS, Mishra BP and Joshi BK(2012) Milk proteins and human health: A1/A2 milk hypothesis. Indian Journal of Endocrinology Metabolism,16(5):856.
6. Bhopale JJ, Chauhan DS and Thorat BN(2015) Studies on effect of period and season on lactation milk yield in Holstein Friesain× Deoni interse crossbred cattle in Maharashtra. International Journal of Tropical Agriculture.33(2 (Part II)):643-647.
7. Lowry OH, Rosebrough NJ, Farr Al and Randall RJ(1951) Protein measurement with the Folin phenol reagent. Journal of Biological Chemistry, 193(1), 265-275
8. Kamizake NK, Gonçalves MM, Zaia CT and Zaia DA (2003) Determination of total proteins in cow milk powder samples: a comparative study between the Kjeldahl method and spectrophotometric methods. Journal of Food composition and analysis, 16(4), 507-516.
9. Khan ZI, Ashraf M, Hussain A, McDowell LR, Ashraf MY(2006) Concentrations of minerals in milk of sheep and goats grazing similar pastures in a semiarid region of Pakistan. Small Ruminant Research,65(3):274-278.
10. Sodhi M, Mukesh M, Kataria RS, Mishra BP and Joshi BK(2012) Milk proteins and human health: A1/A2 milk hypothesis. Indian Journal of Endocrinology Metabolism,16(5):856.
11. Araújo TP, Rangel AH, Lima GF, Peixoto MG, Urbano SA, Bezerra JD(2018) Gir and Guzerat cow milk production and composition according to lactation stage, somatic cell count, physiological state and body condition. Acta Scientiarum. Animal Sciences,40.

Table-1 Estimation of protein by Lowry'method of six different cows

SL NO.	Test Tubes	Distilled water (ml)	Conc. of stock solution(ml)	Reagent C (ml)	Reagent D (ml)
1	1st	1	0	5	0.5
2	2nd	0.8	0.2	5	0.5
3	3rd	0.6	0.4	5	0.5
4	4th	0.4	0.6	5	0.5
5	5th	0.2	0.8	5	0.5
6	6th	0	1	5	0.5

Table 2 Trace elements present in milk samples of different breds of cow

Elements in Milk sample	Different breeds of cows					
	Jersey	Hariana	Desi	Gir	Holstein	Sindhi
Si	200.0 ppm	249.1ppm	242.0 ppm	235.2 ppm	180.9 ppm	
P	0.178 %	0.172 %	0.136 %	0.153 %	0.180 %	0.158%
S	741.6 ppm	619.4ppm	539.9ppm	551.0 ppm	716.5 ppm	516.2ppm
Cl	0.120%	0.113%	573.3%	0.152%	0.130%	0.156 %
K	0.177%	0.191%	0.153%	0.160%	0.171%	0.187%
Ca	0.188%	0.159%	0.157%	0.164%	0.183%	0.147%
Fe	16.4ppm	17.9ppm	16.3ppm	13.5ppm	16.8ppm	13.5Ppm
Co	0.0ppm		0.0ppm	0.0ppm	0.0ppm	8.2Ppm
Zn	8.4 ppm	6.0ppm	3.3 ppm	4.3ppm	8.3ppm	4.9Ppm
Rb	6.4 ppm	6.2 ppm	3.5ppm	5.0 ppm	7.0ppm	7.4 Ppm
Tb	30.0 ppm					
Er	82.2ppm		101.4ppm	67.9ppm	64.3ppm	
Re	0.8ppm	0.8 ppm	0.8 ppm	1.0ppm	1.3ppm	1.5Ppm
H_2O	99.228%	99.270%	99.403%	99.275%	99.228%	99.288%
Sn		49.8ppm		55.6 ppm	53.1ppm	54.9Ppm
Mn			7.0 ppm	4.1 ppm	8.3 ppm	1.9 Ppm
Eu			24.0 ppm	27.1ppm		29.6 Ppm
Gd					33.8 ppm	
Normalisation Factor	1.545	1.566	1.539	1.546	1.211	1.283

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RESEARCH ARTICLE

Synthesis and Characterization of MgO Nanostructures

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ABSTRACT

Here different MgO nanostructures were synthesized by using three different chemical methods such as hydrothermal, reflux and co-precipitation. The interesting thing of these different synthetic methods is to achieve three different morphology of MgO. To confirm the phase, formation and morphology, different characterization methods are used. From XRD, the MgO phase formation was confirmed by different peaks with different inter planar spacing values. The XRD results reveal the well crystalline nature of the prepared compounds. The formation of nanoflakes, hierarchical nanostructure and nanorods wre obtained by hydrothermal, reflux and precipitation methods which were confirmed from FE-SEM images.

Keywords: Nanostructures, MgO, Chemical method, Hydrothermal, Reflux, Precipitation

INTRODUCTION

There are various methods for the fabrication of nanomaterials which are grouped into three main categories: Physical, chemical and biological methods. The physical methods are electric arc discharge, flame pyrolysis, ball milling, laser ablation. Chemical methods include sol-gel, microemulsions, hydrothermal, microwave, co-precipitation and sonochemical methods. The biological synthesis is the greener synthesis includes the use of microorganisms eukaryotes (yeasts, fungi)or prokaryotes (bacteria, actinomycetes), use of plant extracts and enzymes or by the use of templates like diatoms, viruses and membranes [1-10]. Among the several chemical methods the co-precipitation method is the simplest and low cost method widely used for the synthesis of nano level materials [11]. This method can be carried out under very low temperatures and can give nanomaterials of both crystallinity and larger surface areas. In this process first the starting precursors were stirred and mixed together and again it was stirred to form a homogenous mixture. In this method it is important to maintain the purity of the precipitate, thermogravimetric analysis shows that the precipitates contain undesired impurities which can increase

the mass, this can be solved by digestion or by redissolving the precipitates again [12-16]. Sol–gel method is a bottom up synthetic approach, which occours in a 3- D confinement in the liquid phase. In this process the starting solution (sol) undergoes a transition state to form a gel like network containing both solid and liquid phase [16-20]. The starting precursors for this process were generally metal alkoxides, metal chlorides and metal nitrates. These undergoes hydrolysis and polycondensation reaction to form colloids and then it was allowed for sedimentation. Formation of metal oxides involves connecting the metal centers with oxo (M-O-M) [15] or hydroxo (M-OH-M) bridges, hence generating metal-oxo or metal-hydroxo polymers in solution. This method has high advantage over others as it possesses high chemical purity, high range of homogeneity, lower temperature for calcinations and control over particle morphology [21-25].

Hydrothermal synthetic method is a method of production of different chemical compounds and materials in solution phase under high temperatures >600^{0}C and pressures upto 300 MPa. The main parameters including in the hydrothermal synthesis are kinetics, properties of resultant products, initial pH, time interval, temperature and pressure. The term hydrothermal was originated from geology, which produces single crystals [25-30]. The growth of crystals can be done by an apparatus consisting of steel vessel known as autoclaves which can bear high temperatures and pressures for a longer periods. Advantages of this technique are to synthesize crystals of substances that are unstable near the melting point and synthesis of large crystals of high quality. Some of the disadvantages include high cost of the equipments and the in ability to monitor the crystals in the growth process [30-32].

Magnesium oxide is known as magnesia occours naturally as periclase. It is a white hygroscopic solid mineral consisting of Mg^{2+} and O^{2-}ions held by ionic bonding. Its melting point is about 2852^{0}C and boiling point is 3600^{0}C. Due to its high melting pointit is used as insulator windows, limiters and optical beams [33]. It is soluble in acid, ammonia but in soluble in alcohol. MgO have thermal conductivity of 40–60 $Wm^{-1}K^{-1}$, refractive index of 1.73. The crystal structure of MgO is periclase, which contains octahedral Mg^{2+} and O^{2-} ions. Magnesium oxide is a class II-IV semiconductor compound possessing a large band gap of 7.8eV, large dielectric constant of 9.8 and small exciton binding energy less than 0.1eV. Generally magnesia occours in three crystallographic structrures such as rock salt NaCl (B_1), CsCl (B_2) and inverse NiA ($B8_1$). In normal conditions the B_2 and $B8_1$ structures are less stable but with the increase in pressure around 2.2Mbar the $B8_1$ structure is the most stable [34-36]. MgO is focused very much on research area due to their novel properties and wide applicability also it possesses low weight and non-toxic. Synthesis of MgO nanostructured materials of different morphologies like rods, tubes, wires have been paid attention worldwide due to their wide band gap, insulating behavior, piezo and pyro electric properties etc [30-39].
So in this work our man research objectives are synthesis of magnesium oxide nanomaterials of different morphologies by chemical methods such as precipitation, reflux and hydrothermal method and Characterization of synthesized nanomaterial by different scattering and microscopic techniques like XRD, FESEM, FTIR etc.

MATERIALS AND METHODS

Materials Used

Magnesium chloride ($MgCl_2.6H_2O$), ammonium carbonate $(NH_4)_2.6H_2O$) were parched from Merck India. All chemicals are used as such. The double distilled water was used throughout the experiments.

Synthesis of MgO nanoflakes

Hydrothermal method was used for the synthesis of MgO nanoflakes. In this method 4 gm of $MgCl_2.6H_2O$ was taken in a beaker which has 50mL of distilled water. Then stirred for 5min followed by addition of 6 gm of $(NH_4)_2CO_3$. Then the resulting mixture was put in a container followed by hydrothermal treatment for 3hr at 120^{0}C. Then obtained mixture was washed several time with distilled water and dried at 70 °C for 3 hours followed calcined at 400°C for 3 hours form MgO nanoflakes.

Synthesis of MgO nanorods

Co-precipitation method was used for the synthesis of MgO nanorods. In this method 4 gm of $MgCl_2.6H_2O$ was taken in a beaker which has 50mL of distilled water. Then stirred for 1h followed by addition of 6 gm of $(NH_4)_2CO_3$ to obtain white precipitation . Then the resulting precipitation was washed several time with distilled water and dried at 70 °C for 3 hours followed calcined at 400°C for 3 hours form MgO nanorods.

Synthesis of MgO hierarchical nanostructures

Reflux method was used for the synthesis of MgO hierarchical nanostructures. In this method 4 gm of $MgCl_2.6H_2O$ was taken in a beaker which has 50mL of distilled water. Then stirred for 1h followed by addition of 6 gm of $(NH_4)_2CO_3$ to obtain white precipitation . Then the mixture was taken in a round bottomed flask and refluxed for 3 hr at 120 ^{0}C. Then the resulting precipitation was washed several time with distilled water and dried at 70 °C for 3 hours followed calcined at 400°C for 3 hours form MgO hierarchical nanostructures.

Characterization Techniques

The instruments were used for characterization are XRD, SEM and FTIR. Powder X-ray diffraction patterns of the samples were recorded in a PANalytical X-ray diffractometer. It is used to analyse the phase of the sample. Surface morphology, microstructure and particle size of the as obtained samples were studied by Nano Nova 450 *Field Emission*scanning electron microscopy (FE-SEM). The working voltage was kept at 15kV and 20 kV. X-ray scanning used to measure the elemental distribution (EDX).

RESULTS AND DISCUSSION

Surface Morphology and Microstructure

The surface morphology of the as synthesized magnesium carbonates by different chemical methods before calcinations were analyzed by scanning electron microscope and the images were shown below figure 1. Fig 1 (a) shows the formation of $MgCO_3$ nanorods prepared by simple co-precipitation method and are uniformly distributed, Fig. 1 (b) shows the formation of hierarchical morphology prepared by reflux method and Fig 1 (c) shows the formation of flakes like nanostructures synthesized under hydrothermal method. The above $MgCO_3$ prepared by 3 different chemical methods were calcined at 400 ^{0}C for 3 hr to form MgO nanomaterials. Fig. 1(e) shows the EDAX spectra of MgO synthesized by reflux method. From this spectrum, it is confirmed that the presence of Mg and O elements.

X-ray Diffraction Analysis

The X-ray diffraction patterns of as synthesized and calcined samples of magnesium oxide (MgO) nanomaterials prepared under different wet chemical methods were shown below.

Nanoflakes

The XRD pattern of MgO nanoflakes before and after calcination which were synthesized from hydrothermal method represents in Fig. 2. From this spectra, a mixture of monoclinic and orthorhombic phases are confirmed according to JCPDS no 25-0513 and 70-1177. Again from Fig.2 (b) confirmed the formation MgO with JCPDS no 78-0430 after calcination [30-35].

Hierarchical Nanostructure

The XRD pattern of MgO hierarchical nanostructure before and after calcination which were synthesized from reflux method represents in Fig. 3. From this spectra, a mixture of monoclinic and orthorhombic phases are confirmed according to JCPDS no 25-0513 and 70-1177. Again from Fig.3 (b) confirmed the formation MgO with JCPDS no 78-0430 after calcination [35-39].

Nanorods

The XRD pattern of MgO nanorods before and after calcination which were synthesized from precipitation method represents in Fig. 4 (a). From this spectra, a mixture of artinite and monoclinic phases are confirmed according to JCPDS no 70-0591. Again from Fig.4 (b) confirmed the formation MgO with JCPDS no 78-0430 after calcination [30-34].

CONCLUSIONS

Here different MgO nanostructures were synthesized by using three different chemical methods such as hydrothermal, reflux and co-precipitation. The interesting thing of these different synthetic methods is to achieve three different morphology of MgO. To confirm the phase, formation and morphology, different characterization methods are used. From XRD, the MgO phase formation was confirmed by different peaks with different inter planar spacing values. The XRD results reveal the well crystalline nature of the prepared compounds. The formation of nanoflakes, hierarchical nanostructure and nanorods wre obtained by hydrothermal, reflux and precipitation methods which were confirmed from FE-SEM images.

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REFERENCES

1. H. R. Mahmoud, S. A. E Molla and M. Saif, Powder Technology, 249 (2013) 225–233.
2. S. U. Bayca, M. F. Cansizoglu, A. S. Biris, F. Watanabe and T. Karabacak, int. jour. Ofhyd. Energy, 36 (2011) 5998-6004.
3. W. J. Park, M. H. Kim, B. H. Koo, W. J. Choi, J.L. Lee and J. M. Baik, Sensors and Actuators: B, 185 (2013) 10–16.
4. R. Murugan , K.Ramamoorthy , S. Sundarrajan and S. Ramakrishna, Tetrahedron, 68 (2012) 7196-7201.
5. J. H. Ferrer, P. Laporta, F. Gutiérrez, M. D. Rubianes, G. Rivas and M.T. Martínez, Electrochemistry Communications, 39 (2014) 26–29.
6. R. Sathyamoorthy, K.Mageshwari, S.S. Mali, S.Priyadharshini and P. S.Pati, Ceramics International, 39 (2013) 323–330.
7. V. Stengl, S. Bakardjieva, M. Marikova, P. Bezdicka and J. Subrt, Materials Letters, 57 (2003) 3998–4003.
8. J. Huang, Y. Cao, Z. Liu, Z. Deng, F. Tang and W. Wang, Chemical Engineering Journal, 180 (2012) 75– 80.
9. Y. Su, H. Wei, Z. Zhou, Z. Yang, L. Wei and Y. Zhang, Materials Letters, 65 (2011) 100–103.
10. H. Li, M. Li, X. Wang , X. Wu , F. Liu and B. Yang, Materials Letters, 102 (2013) 80–82.
11. Y. Liu, G. Wang, J. Zhao, L. Jiang, S. Fang and Y. Sun, Colloids and Surfaces A: Physicochem. Eng. Aspects, 426 (2013) 12–17.
12. Y.Aykut, Jour. of Phys. and Chem. of Solids, 74 (2013) 328–337.
13. N. Pugazhenthiran, S. Ramkumar, P. Sathish Kumar and S. Anandan,Microporous and Mesoporous Materials, 131 (2010) 170–176.
14. EAde Boer, L.D. Bell, M.L.Brongersma, H.A. Atwater, M.L.Ostraat and R.C.Flagan.Appl. Phys.Lett, 78(2001)3133-5.
15. D. Zhao, Y. Zhu, R. Li and J. Liu, Solid-State Electronics, 49 (2005) 1974–1977.
16. DV.Talapin, JS. Lee, MV.Kovalenk, EV. Shevchenko,Chem Rev 110(2010) 389-458.
17. MC Daniel and D.Astruc, Chem. Rev,104 (2004) 293-346.
18. ZGu, T. Zhai, BGao, , X Sheng, Y. Wang, H. Fu, , Y. Ma and J. Yao, J. Phys. Chem. B,110(2006) 23829.
19. F Lu, W. Cai and Y Zhang,Adv. Funct. Mater, 18 (2008) 1047.

20. T Zhang, WDong, M.Keeter-Brewer, K.Sanjit, R. NNjabon and Z. RTian,J. Am.Chem. Soc, *128* (2006) 10960.
21. CD Dimitrakopoulos and PRL Malenfant, Advanced Materials, 14 (2002) 99-117.
22. A.K. Hall, S.A. Rowlands, P.G. McCormick, R. Street, R.J. Hart, G.F. Ebell and P. Donecker, Destruction of toxic materials, Nature, 367 (1994) 223.
23. H. Wang, J. Huang, K. Zhang, Y. Yu, K. Liu, G. Yu, S. Deng and B. Wang,Journal of Hazardous Materials, 264 (2014) 230– 235.
24. X. Fu, Y. Hu, Y. Yang, W. Liu, S. Chen, Journal of Hazardous Materials 244– 245 (2013) 102– 110.
25. R. Strobel and S.E. Pratsinis, J. Mater. Chem, 17 (2007) 4743–4756.
26. M. Høja, K. Lindea, T. Hansena, M. Brorsonb, A. D.Jensena,J.D.Grunwaldt Applied Catalysis A: General 397 (2011) 201–208.
27. P.Pawinrata, O.Mekasuwandumrong and J.Panpranot, Catalysis Communications, 10 (2009) 1380–1385.
28. L. Tonks andI. Langmuir, Phys. Rev, 33 (1929) 195.
29. Z. Petrovic and T. Makabe, Adv. Mater.Proc, 282 (2) (1998) 47–56.
30. A. Matsuda, J. Vac. Sci. Technol. A: Vac. Surf. Films, 16 (1) (1998) 365–368.
31. C. Benndor, P.Joeris and R. Kroger, Pure Appl. Chem, 66 (6) (1994) 1195–1205.
32. H. Biederman and Y. Osada, Plasma chemistry of polymers Adv. Polym.Sci, 95 (1990) 57–109.
33. W. Jiang, X. Hua, Q. Han, X. Yang, L. Lu and X. Wang, Powder Technology, 191 (2009) 227–230.
34. F. Gu, S. Wang, M. Lu, G. Zhou, D. Xu and D. Yuan, J. Phys. Chem. B, 108(2004), 8119-8123.
35. J. Gray and B. Luan, J. Alloys Compd,. 336 (2002) 88–113.
36. Y. Zhu, Q. Zhao, Y. Zhang and G. Wu, Surface & Coatings Technology, 206 (2012) 2961–2966.
37. N. Nga, P. T.Honga, T. D. Lamb and T. Q.Huy, Journal of Colloid and Interface Science, 398 (2013) 210–216.
38. F. Al-Hazmi, F. Alnowaiser, A. Al-Ghamdi , A. Al-Ghamdi, M. M. Aly, R. M. Al-Tuwirqi and F. El-Tantawy, Superlattices and Microstructures, 52 (2012) 200–209.
39. Y.Zhanga, M. Ma, X. Zhanga, B.Wanga and R. Liu,Journal of Alloys and Compounds, 590 (2014) 373–379.
40. W. Wang, X. Qiao, J. Chen and H. Li,Materials Letters, 61 (2007) 3218–3220.
41. Z. Zhang, Y. Zheng, J. Chen,Q. Zhang, Y. Ni andX. Liang, Adv.Funct. Mater,17 (2007) 2447–2454.
42. M. Rezaei, M. Khajenoori and B.Nematollahi,Materials Research Bulletin, 46(2011) 1632–1637.
43. K. Mageshwari and R. Sathyamoorthy,Trans. Indian Inst. Met, 65(1)(2012) 49–55.
44. F. Al-Hazmi, F. Alnowaiser, A. Al-Ghamdi , A. Al-Ghamdi, M.M. Aly, R. M. Al-Tuwirqi and F. El-Tantawy,Superlattices and Microstructures, 52 (2012) 200–209.

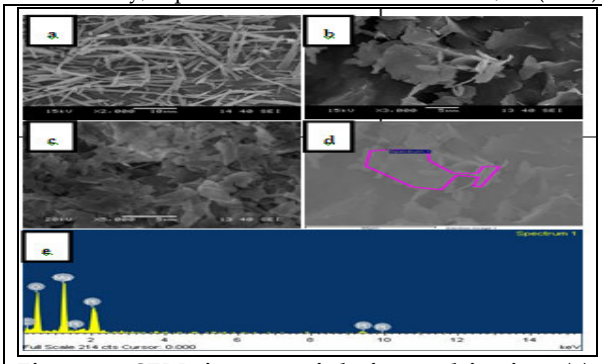

Fig. 1 : SEM images of before calcination (a) precipitation method, (b) reflux method (c) hydrothermal method (d) EDAX image of reflux method.

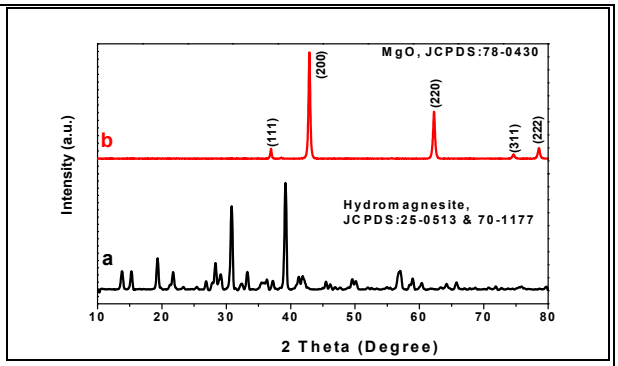

Fig. 2 : XRD MgO synthesized by hydrothermal method (a) before calcination, (b) after calcination

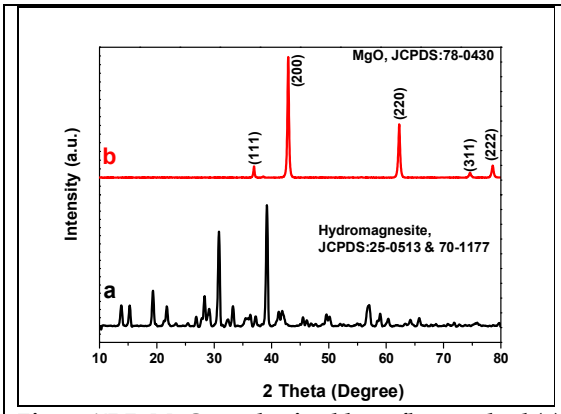

Fig. 3 : XRD MgO synthesized by reflux method (a) before calcination, (b) after calcination

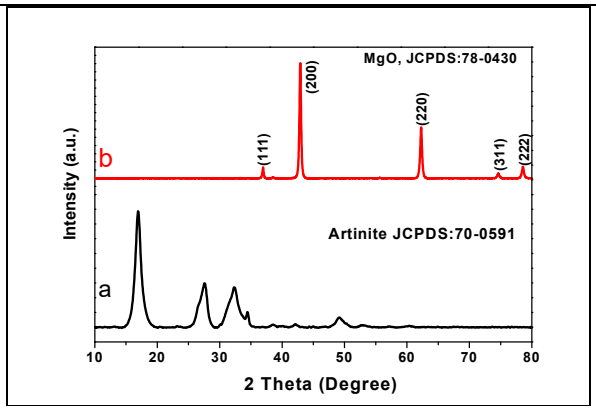

Fig. 4: XRD MgO synthesized by precipitation method (a) before calcination, (b) after calcination

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RESEARCH ARTICLE

Synthesis and Characterization of MgO-Fe_2O_3NanocompositeUsing Precipitation Method

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ABSTRACT

In this project, we have synthesized MgO-Fe_2O_3nanocompositesthrough precipitationmethod using magnesium nitrate and ferric nitrate as salt precursors. Here polyethylene glycol and NaOH were stabilizing and precipitating agents respectively. Apart from this we have also synthesize pristine MgO, Fe_2O_3nanoparticles using the same synthetic method for comparison study. In order to determine the information on the crystal structure, formation, size, and morphology of the prepared nanocomposite were characterized by using XRD and FESEM analytical techniques.

Keywords: Nanocomposites, Precipitation, Iron, Magnesium

INTRODUCTION

Nanocomposites can be defined as the composite material of which at least one phase has dimensions of less than 100 nanometers. It is consists of solid or bulk material matrix with nano-dimensional phases of one, two or more nanomaterials. Arrangement of nanomaterials is random in nanocomposites [1-3]. High surface to volume ratio of reinforcing phases of nanocomposites, differentiate nanocomposites from conventional composite materials. The reinforcing material can be made up of nanomaterials like nonaparticles, nanofibers, nanosheets. The matrix material is affected by proximity of reinforcement [4]. A small amount of nanoscale reinforcement gives a huge effect (i.e observable effect) on macroscalepropertiesof the composites due to the large amount of reinforcement surface area. They have a huge range of applications on medicines, microelectronics, nanophotonics, sensors, food packaging, cosmetics. Nanocomposites are tools of nanotechnology which show a great change in all industrial fields [5-10].Nowadays metal Oxide nanomaterials can have much more attraction in various fields due to their important properties [11,12].

Nanomaterials can be synthesized by various chemical methods like hydrothermal, co-precipitation and sol-gel.Among the several chemical methods the co-precipitation method is the simplest and low cost method widely used for the synthesis of nano level materials [13]. This method can be carried out under very low temperatures and can give nanomaterials of both crystallinity and larger surface areas. In this process first the starting precursors were stirred and mixed together and again it was stirred to form a homogenous mixture. In this method it is important to maintain the purity of the precipitate, thermo gravimetric analysis shows that the precipitates contain undesired impurities which can increase the mass, this can be solved by digestion or by redissolving the precipitates again. Hence here we have synthesized mixed iron and magnesium oxides nanocomposite through simple and cost effective precipitation method [14-15].

MATERIALS AND METHOD

Materials

$Mg(NO_3)_2$. $6H_2O$,$Fe_2(NO_3)_3$. $9H_2O$, NaOH and Polyethylene glycol, Congo redwere purchased from sigma Aldrich. Ethanol is purchased from Merck chemicals Ltd.India

Preparation of MgO nanomaterial

2.56g of $Mg(NO_3)_2.6H_2O$ and 2.56g of PEG and 25mL of ethanol was added to a beaker. The mixture was stirred in 50-60^oC till a clear solution appears. Then NaOH was added drop wise till the pH become 11-12 with continuous stirring for 6h to formed whitish precipitation. Then obtained precipitation was kept in air oven for 12hrs at 150^oC to dry followed by calcination at 550^oC to obtain desired product.

Preparation of Fe_2O_3 nanomaterial

4g of $Fe(NO_3)_3$. $9H_2O$ and 4g of PEG and 25mL of ethanol were mixed in a beaker. The mixture was stirred continuously in 50-60^oC till a clear solution appears. Then NaOH was added drop wise and made the pH of the solution in range of 11-12. Then obtained brown precipitation was kept in air oven for 12hrs at 150^oC to dry followed by calcination at 550^oC to obtain Fe_2O_3nanomaterilas.

Preparation of MgO-Fe_2O_3nanocomposite

Different weight ratios of MgO-Fe_2O_3 were synthesized by hydrothermal method by taking $Mg(NO_3)_2$. $6H_2O$ and $Fe(NO_3)_3$. $9H_2O$ with PEG and alcohol in a beaker. Stirred the above mixture in 50-60^oC till a clear solution appears. Then NaOH was added drop wise so that pH of the solution is in the range of 11-12. Then obtained whitish brown precipitation was kept in air oven for 12hrs at 150^oC to dry followed by calcination at 550^oC to obtain desired product.

Characterization techniques

To confirm the formation and morphology of synthesized nanomaterials we have used various analytical methods. The instruments were used for characterization are XRD and SEM. Powder X-ray diffraction patterns of the samples were recorded in a PAN alytical X-ray diffractometer. It is used to analyze the phase of the sample. Surface morphology, microstructure and particle size of the as obtained samples were studied by Nano Nova 450 *Field Emission*scanning electron microscopy (FE-SEM). The working voltage was kept at 15kV and 20 kV. X-ray scanning used to measure the elemental distribution (EDX).

RESULT AND DISCUSSION

Xrd Analysis

The phase analysis of the prepared nanocomaterials was analyzed by XRD using CuKα radiation. Fig. 1 shows the XRD patterns of the as preparedMgO, α-Fe_2O_3 nanoparticles and α-Fe_2O_3-MgO nanocomposite. The pattern (a) contains the characteristics peaks of MgO and can be index to cubic crystal structure according to JCPDS No: 45-0946. The pattern (b) contains characteristics peaks of hematite (α-Fe_2O_3) and can be index to rhombohedral crystal structure according to JCPDS No: 24-0072. The pattern (c) contains the characteristics peaks of both MgO andα-Fe_2O_3. The X-ray diffractograms reveal the well crystalline nature of the compounds.

Surface Morphology

In order to understand the morphologies of our nanocomposites, FESEM analysis was performed. Fig. 2(a) and 3(b) shows the FESEM images of α-Fe_2O_3-MgO nanocomposite. This image indicates that there is formation of fine nanoparticles with average diameter range 50-80nm.Figures 2(c) and 2(d) shows the EDX elemental mapping and EDX spectra of α-Fe_2O_3-MgO nanocompositerespectively, in which presence of Fe, Mg and O is indicated.

CONCLUSIONS

MgO-Fe_2O_3 nanocomposite was synthesized through precipitation method using magnesium nitrate and ferric nitrate as salt precursors. Here polyethylene glycol and NaOH were stabilizing and precipitating agents respectively. Apart from this we have also synthesize pristine MgO, Fe_2O_3 nanoparticles using the same synthetic method for comparison study. In order to determine the information on the crystal structure, formation, size, and morphology of the prepared nanocomposite were characterized by using XRD and FESEM analytical techniques.

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REFERENCES

1. R.K. Upadhyay, N. Soin, S.S. Roy, Role of graphene/metal oxide composites as photocatalysts, adsorbents and disinfectants in water treatment: A review, RSC Adv. 4 (2014) 3823–3851. https://doi.org/10.1039/c3ra45013a.
2. B.H. Hameed, A.A. Rahman, Removal of phenol from aqueous solutions by adsorption onto activated carbon prepared from biomass material, J. Hazard. Mater. 160 (2008) 576–581. https://doi.org/10.1016/j.jhazmat.2008.03.028.
3. L.D. Nguyen, S. Gassara, M.Q. Bui, F. Zaviska, P. Sistat, A. Deratani, Desalination and removal of pesticides from surface water in Mekong Delta by coupling electrodialysis and nanofiltration, Environ. Sci. Pollut. Res. (2018).
4. A.I.A. Sherlala, A.A.A. Raman, M.M. Bello, A. Asghar, A review of the applications of organo-functionalized magnetic graphene oxide nanocomposites for heavy metal adsorption, Chemosphere. 193 (2018) 1004–1017. https://doi.org/10.1016/j.chemosphere.2017.11.093.
5. S.K. Sahoo, G. Hota, Surface functionalization of GO with MgO/MgFe2O4binary oxides: A novel magnetic nanoadsorbent for removal of fluoride ions, J. Environ. Chem. Eng. 6 (2018) 2918–2931. https://doi.org/10.1016/j.jece.2018.04.054.
6. M. Hossein, H. Alijani, Y. Fazli, Solvent free synthesized MnFe 2 O 4 @ polyamid resin as a novel green nanohybrid for fast removing Congo red, J. Mol. Liq. 216 (2016) 6–11.

https://doi.org/10.1016/j.molliq.2016.01.017.

7. T. Hao, C. Yang, X. Rao, J. Wang, C. Niu, X. Su, Applied Surface Science Facile additive-free synthesis of iron oxide nanoparticles for efficient adsorptive removal of Congo red and Cr (VI), Appl. Surf. Sci. 292 (2014) 174–180. https://doi.org/10.1016/j.apsusc.2013.11.108.
8. T. Hao, X. Rao, Z. Li, C. Niu, J. Wang, X. Su, Synthesis of magnetic separable iron oxide / carbon nanocomposites for efficient adsorptive removal of Congo red, J. Alloys Compd. 617 (2014) 76–80. https://doi.org/10.1016/j.jallcom.2014.07.111.
9. R. Lafi, K. Charradi, M. Amine, A. Ben, H. Amara, A. Hafiane, Adsorption study of Congo red dye from aqueous solution to Mg – Al – layered double hydroxide, Adv. POWDER Technol. (2015). https://doi.org/10.1016/j.apt.2015.12.004.
10. S. Zhao, D. Chen, F. Wei, N. Chen, Z. Liang, Y. Luo, Ultrasonics - Sonochemistry Removal of Congo red dye from aqueous solution with nickel-based metal- organic framework / graphene oxide composites prepared by ultrasonic wave-assisted ball milling, Ultrason. - Sonochemistry. 39 (2017) 845–852. https://doi.org/10.1016/j.ultsonch.2017.06.013.
11. L. Ren, H. Lin, F. Meng, F. Zhang, One-step solvothermal synthesis of Fe 3 O 4 @ Carbon composites and their application in removing of Cr (VI) and Congo red, Ceram. Int. (2018) 0–1. https://doi.org/10.1016/j.ceramint.2018.11.132.
12. C.M. Babu, R. Vinodh, B. Sundaravel, A. Abidov, M.M. Peng, W.S. Cha, H.T. Jang, Characterization of reduced graphene oxide supported mesoporous Fe2O3/TiO2 nanoparticles and adsorption of As(III) and As(V) from potable water, J. Taiwan Inst. Chem. Eng. 62 (2016) 199–208. https://doi.org/10.1016/j.jtice.2016.02.005.
13. M. Barathi, A.S. Krishna Kumar, C.U. Kumar, N. Rajesh, Graphene oxide–aluminium oxyhydroxide interaction and its application for the effective adsorption of fluoride, RSC Adv. 4 (2014) 53711–53721. https://doi.org/10.1039/C4RA10006A.
14. Y. Cao, X. Li, Adsorption of graphene for the removal of inorganic pollutants in water purification□: a review, Adsorption. 20 (2014) 713–727. https://doi.org/10.1007/s10450-014-9615-y.
15. M. Chen, Y. Sun, C. Huo, C. Liu, J. Wang, Akaganeite decorated graphene oxide composite for arsenic adsorption / removal and its proconcentration at ultra-trace level, Chemosphere. 130 (2015) 52–58. https://doi.org/10.1016/j.chemosphere.2015.02.046.

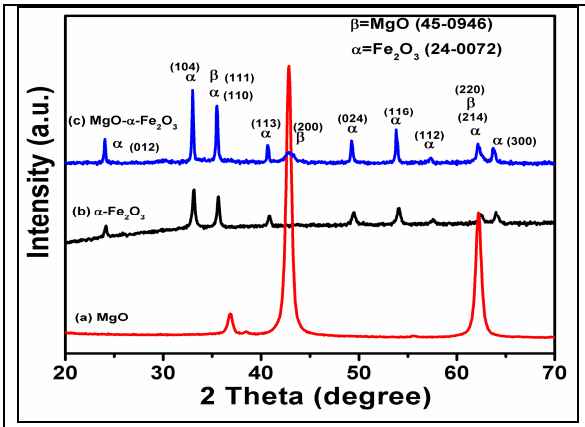

Fig. 1. XRD patterns of (a) MgO, (b) α-Fe_2O_3 nanoparticles and (c) α-Fe_2O_3-MgO nanocomposite.

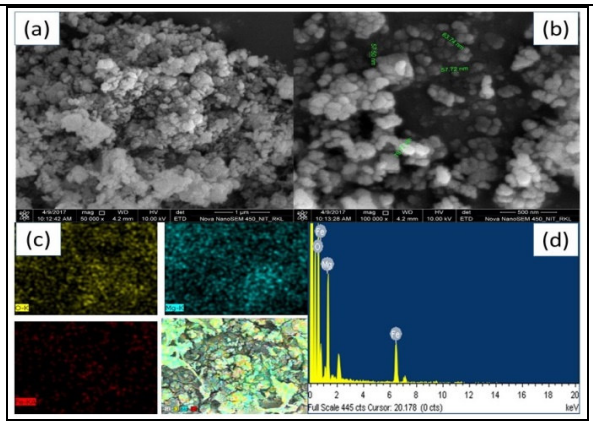

Fig. 2. FESEM image of (a) and (b) α-Fe_2O_3-MgO nanocomposite, (c) EDS elemental mapping and (d) EDX spectra of α-Fe_2O_3-MgO nanocomposite.

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RESEARCH ARTICLE

Effect of pH on the Removal of Congo Red Dye Using MgO Nanoparticles

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ABSTRACT

Here, we have synthesized MgO nanomaterial by using costefficiftive and simple precipitation method using magnesium nitrate as starting material and polyethylene glycol as stabling agent where sodium hydroxide is precipitating agent. Then the synthesized nanomaterial was used for the removal of highly toxic Congo red (CR) dye from water by changing pH of the solution. From the results, it was confirmed maximum adsorption occurs at pH=7.

Keywords: Magnesium, Nanoparticles, Co-precipitation, Adsorption, Congo red

INTRODUCTION

Nanoscience is the study of properties and phenomena of nanoscale materials. Nanomaterials are materials which are made of grains in the size range of 1-100 nanometer (nm). 1nm comprise 10 Å [1]. Nanomaterials are those materials having at least one of their dimensions at nanoscale range. Nanomaterials can be of zero dimension (e.g., nanoparticles), one dimension (e.g., nanofibers, nanotubes, nanorods, nanowires), two dimensions (e.g., nanofilms, nanolayers, nanocoatings), or three dimensions (e.g., dispersion of nanoparticles, rolls of nanowires, and nanotubes) [1–3]. Materials like graphene, thin films, or surface coatings are two dimensional nanomaterials. The main two factors that increase the properties of nanomaterials compare to other materials are high specific surface area, and quantum dimension effects. These factors can change the properties of nanomaterials such as high electrical properties, reactivity, strength and optical properties [4]. Nano sized materials have created a great interest in chemistry, physics, bioscience and engineering in recent years because of their unusual mechanical, electrical, optical and magnetic properties. These unique properties make them as potential candidates for commercially used purposes like adsorption, catalysts, photocatalysts, fillers, electronic, drug delivery, energy storage and fillers [2–4].

Congo red (CR) (disodium 4-amino-3-[[4-[4-[(1-amino4-sulfonatonaphthalen-2-yl) diazenyl] phenyl] phenyl] diazenyl] - naphthalene-1-sulfonate) is a benzidine based anionic dye. It is generated from textiles, printing and dyeing, paper, rubber and plastics industry, among others. CR is known to metabolize into benzidine, which is a known human carcinogen Therefore, it is very important to remove residual Congo red from water sources before discharge to receiving water bodies. Treatment of wastewater containing dyes is conventionally done by several physicochemical and well as biological methods including coagulation-flocculation, advance oxidation, adsorption, ozonation, photo-chemical degradation, fungal decolorization, etc. However, adsorption is the most popular method among the aforementioned ones due to its low operational cost, low maintenance and simplicity [5-10].
The main objectives of this work are:

- To synthesize MgOnanomaterials by using cost effective method.
- To characterize the synthesized nanomaterials using XRD and FTIR
- To remove the CR dye by adsorption

MATERIALS AND METHODS

Materials

All of the chemicals were of analytical grade and used without further purification. Graphite powder (300 mesh), Poly ethylene glycol (PEG; Mn=20,000), Magnesium nitrate hexahydrate($Mg(NO_3)_2.6H_2O$) were bought from Sigma Aldrich (USA). Ethanols (C_2H_5OH), Sodium Hydroxide (NaOH) were purchased from Merck (INDIA).

Synthesis of MgO nanomaterial

Co-precipitation method was used to synthesize MgO composite nanomaterials. In this method, $Mg(NO_3)_2.6H_2O$ and polyethylene glycol (PEG; MW: 20,000) were dissolved in 70 mL of ethanol with 1:2 mol ratios of Mg and polymer respectively (where PEG was used for controlling the size of the nanocomposite). Then 2M NaOH was added drop wise to the mixture up to pH 11 under magnetic stirring. After 3h of vigorously stirring, the white precipitated reaction mixture was obtained. After that the prepared sample was washed several times with ethanol and distilled water and then dried at 60^0C for 4 hours. Then the dried sample was calcined at 350^0C for 3hours with heating rate 10^0C /min to form MgOnanomaterials.

Adsorption of Congo Red(CR)

The Dye adsorption efficiencies of the prepared MgOnanomaterials were tested towards adsorption of Congo Red (CR) in an orbital shaker. Initially a stock solution of 1 g of Congo red was dissolved in 1000 ml of double distilled water. In a typical experiment, 0.01 gm of adsorbate were added to20 ml of 100mg/L Congo red solution in a 100 ml of beaker for adsorption. After adsorption the solution was filtered. Then the solution was put into a quartz cell, and adsorption spectrum was measured using Shimadzu UV-2450 spectrometer. The percentage removal can be calculated by the following equation.

Percentage of removal = $\frac{C_0 - C_t}{C_0} X100$ **(1)**

RESULTS AND DISCUSSIONS

Conformation of formation of MgO using XRD

The above figure reveals the XRD patterns of MgO nanomaterial. The XRD pattern of MgO contains characteristics peaks at at 2θ=37.05°, 43.42° and 62.1° belong to the plane (111), (200), and (220) respectively are index to cubic structure of MgO according to JCPDS no. 45-0946.Surface morphology of synthetic MgO nanomaterial was analyzed

by FESEM and represented in Fig. 2. From the figure it is confirmed that the formation of fine nanoparticles with range 50-80 nm.

Effect of pH on CR removal by MgO nanoparticles

The effect of pH is an important controlling parameter on the dye adsorption capacity. Figure 3 shows the adsorption of Congo red dye on different pH for 20 mL of 100 mg L^{-1} each dye. In our study we have taken pH range from 3-8. The adsorption of Congo red dye, a diazo dye having a natural pH of 7.1, It was found that the dye solution becomes dark blue from red when the pH was lowered to 3 but became original colour after some time when it was shaken in the orbital shaker also the red color was changed to slightly red when the pH was above 10–12. Therefore, in this study, the pH of the solution was maintained in between 3-8. The equilibrium adsorption of Congo red was observed in pH 6-7 and then decreases. The maximum % removal of dye was seen by more than 99% at pH 7.

CONCLUSIONS

Here, we have synthesized MgO nanomaterial by using costefficiftive and simple precipitation method using magnesium nitrate as starting material and polyethylene glycol as stabling agent where sodium hydroxide is precipitating agent. Then the synthesized nanomaterial was used for the removal of highly toxic Congo red (CR) dye from water by changing pH of the solution. From the results, it was confirmed maximum adsorption occurs at pH=7.

REFERENCES

1. H. R. Mahmoud, S. A. E Molla and M. Saif, Powder Technology, 249 (2013) 225–233.
2. S. U. Bayca, M. F. Cansizoglu, A. S. Biris, F. Watanabe and T. Karabacak, int. jour. Ofhyd. Energy, 36 (2011) 5998-6004.
3. W. J. Park, M. H. Kim, B. H. Koo, W. J. Choi, J.L. Lee and J. M. Baik, Sensors and Actuators: B, 185 (2013) 10–16.
4. R. Murugan ,K.Ramamoorthy , S. Sundarrajan and S. Ramakrishna, Tetrahedron, 68 (2012) 7196-7201.
5. J. H. Ferrer, P. Laporta, F. Gutiérrez, M. D. Rubianes, G. Rivas and M.T. Martínez, Electrochemistry Communications, 39 (2014) 26–29.
6. R. Sathyamoorthy, K.Mageshwari, S.S. Mali, S.Priyadharshini and P. S.Pati, Ceramics International, 39 (2013) 323–330.
7. V. Stengl, S. Bakardjieva, M. Marikova, P. Bezdicka and J. Subrt, Materials Letters, 57 (2003) 3998–4003.
8. J. Huang, Y. Cao, Z. Liu, Z. Deng, F. Tang and W. Wang, Chemical Engineering Journal, 180 (2012) 75– 80.
9. Y. Su, H. Wei, Z. Zhou, Z. Yang, L. Wei and Y. Zhang, Materials Letters, 65 (2011) 100–103.
10. H. Li, M. Li, X. Wang , X. Wu , F. Liu and B. Yang, Materials Letters, 102 (2013) 80–82.

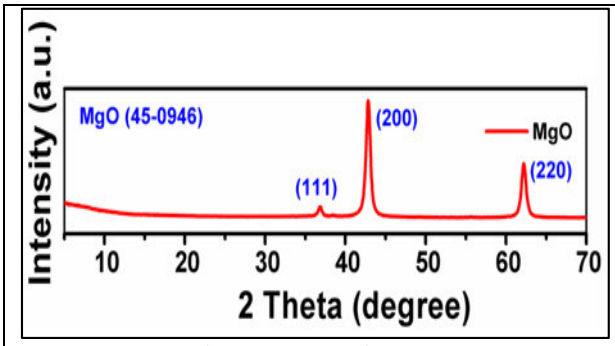

Figure 1: XRD of MgO

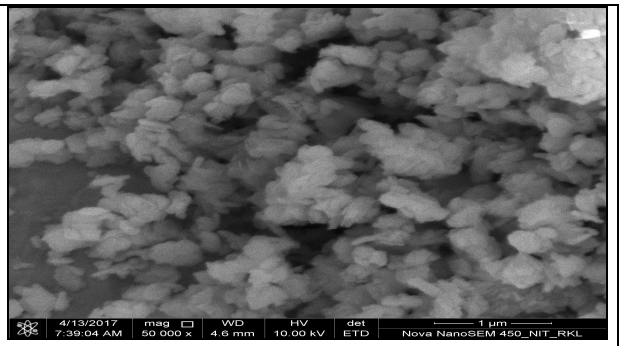

Fig. 2 FESEM Image of MgO nanoparticles

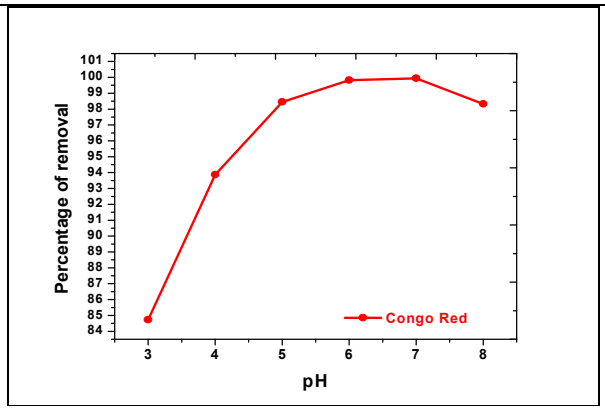

Figure 3: Effect of pH on the removal of Congo red.

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RESEARCH ARTICLE

Bauxite Waste as Cement Substitute after Normalisation: Sustaining Environment

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ABSTRACT

Red mud, the bauxite residue is adiscarded materials producedfrom the Bayer's methodof production ofalumina. The muck is highly alkalising the soil and deteriorating the outskirt ecosystem. The cement plants yield noxious gasses declining the normal geo-bio and hydrosphere.Red mud waste produced in India is ≈70 MMT (0.8 to 1.5Mt per Ton production of alumina). Present work is investigating resemblance of chemical constituent of cement and the red-mud waste by using XRF Spectroscopy.The highly alkaline raw red mud (pH >10) has been normalized by sea water before using as cement substitute. Cubes, cylinders and beams are casted at different Normalized Red Mud (NRM) substitute. The physical and mechanical properties are tested in the laboratory by gadgets like CTM and UTM. The optimum % of NRM substitute of cement was found to be 20% by weight of cement with 5% addition of hydrated lime. The use of red mud, can prevent the water (both surface and ground), the soil, the vegetation and the faunal biodiversity around the Bauxite industry and maintain a sustainable natural environment.

Keywords: Bauxite, Concrete, XRF Spectrometer, UTM, Normalized Red Mud

INTRODUCTION

The Bayer's process employs theabstraction of alumina from the ore, bauxiteis a cost-effective process. The red mud slurry (Bauxite tailings) of the process is generatedcontaining 40-60% of Al_2O_3. The process implicates digestion of ore with caustic soda (NaOH) at raised hotness and mercury to extract alumina and leaving red coloured slurry as residue of high alkalinity called Red mud (RM). The global inventory of Red mud generation of about ≈150MMT/year and India has capacity of generating 9MMT of red mud as per; PTI; Out Look 26th July 2019. China is

the largest producer (54%) of aluminium (Al) (32.6MMT) and largest consumer of alumina (Al_2O_3) of 72 MMT. India (5%)is the fourth producer after USSR (6%) and Canada(%) , has plants with capacity 19.3 MMT of bauxite processing (Data 2015) and 0.6 MMT of crude aluminium metal and producing red mud waste of 2MMT disposing to RM ponds, Samal et al. 2013 [1], Nayak and Mishra 2016 [2], Singh J., 2019 [3]. The state Odisha hasthe highest bauxite reservefollowed by Jharkhand, Maharashtra, MP, and Chhattisgarh.Interestingly AP/Telangana has good amount bauxite reserve but no plants.

Past Spill/breach of RM Lagoon

The breaches/spillage from RM ponds has invited catastrophe in past. Ajka red mud pond breech, 2010 (Hungary), had long term adverse impact on soil and water. As long term impacts; the RM inundated soil /water have turned into highly alkaline (rich in $AL(OH)_4$) and toxic hexavalent Chromium),with growth of new organisms having eco-toxicological genotoxic effects on local vegetation and habitats,(Ruyters et al., 2011[4], Milacic et al., 2012[5], Mayes et al., 2016[6] and Pontius W., 2018[7]).During 8/ 2016, the RM waste pond breach had inundated Dahegou and Luoyang villages of Henan Province in China and resulted heavy crop loss. The RM Pond at Vedanta Alumina refinery at Lanjipally in Koraput district of Odisha, India is always at risk of breach/spillin RM pond and is of constant threat to the villages nearby during rainy season every year from 2016. The related conservational trepidations related to production of huge quantity of RM waste for disposal and casualties due to breach/ spill during heavy rain is the challenge with Alumina industry. Hence it is pertinent to use the alumina industry residue in an effective and eco-friendly manner to reduce the hazard.

LITERATURE REVIEW

Partial replace of cement (about 20%) with red mud has been tried as RM has Al_2O_3 and Fe_2O_3 similar ingredients and almost equal proportion as that of Portland cement and retain thecementous properties and mechanical strength, (Rathod RR. et al., 2012 [8], SawantB.et al. 2011[9, 10], Metilda D. L. et al. 2015[11], Sarod D., et al, 2015 [12], Gowsalya. R et al 2015(13),Deepika at al., 2017[14], Varghese M., 2017[15], Nayak and Mishra et al., 2017[2] and Das Mohapatra and Mishra et l 2019[16]) and also with other ingredients like ultra-fines (GGBS), fly ash, Meta Kaolin, Rice Husk, Silica Fumes, Menhosh et al., 2017[17}, Kulkarni S 2018[18], Kamaldeep et al. 2019 [19] and Das & Mishra 2020 [19] etc.The RM waste disposal in RM Lagoon /ponds environmental degrading due to high alkalinity (pH>10), GW pollution (NaOH contaminant), leading to health hazards. (Bishetti P.N., et al. 2014[20], Pujar S.M. et al. 2014 [21], Normalization of highly alkaline RM (pH >10) can be normalised (pH <8) by sea water, (Tuazone et al., 2015 [22]). SamalS.et.al (2013)[1]pointed about difference in constituent of red mud of India from other countries.Snigdha et.al.(2008)[23], Riberio et.al (2011) [24], are of opinion that thenormalized red mud cement concrete offer more resistance against the chloride attack by its fillings effects.Three pleat benefits can be attributed to RM like waste disposal, raw material and supplementary values when used as building ingredients such as dyes/paints, bricks/ paver blocks, Pavements Kerbs/shoulders, stalls, sea defences, small bins, sewage pipes, floor tiles and light weight concrete *etc.* (Tauber et.al.,1971[25], Satapathy et al, (1991) [26], , Garg et al., 2015 [27], Lima et.al.,2017 [28]).

Objective

The investigation is conducted to assess (a) The normalisation of red mud with sea water (b) the optimum substitute of cement by RM (red mud) (c) to find physical, chemical, and mechanical characteristics of conventional cement concrete and (d) compare it with different % of blending of made with red mud after normalisation.

METHODS

Recycling and Reuse of RM

To save the ecosystem, soil and water near the alumina industry, the focus should be on reuse of the toxic RM. The Bauxite waste has been utilized as (a) manufacture of cement (Qiu et al., 2011[28], Liu Dong et al., 2012 [29]), (b) Ceramics production (Amritphale et al., 2007 [30]), (c) manufacture of NRM bricks, paints, catalysts *etc.* (Pontikesh et al., 2007[31] and Arhin et. Al., 2013 [32], Busto et al., 2016 [33]), (d) Preparation of Paver blocks as per IS:15658-2006,

(Velumani et al., 2017 [34], Batham G., 2018 [34] [35], Das Mohapatra and Mishra 2020 [19]), (e) Absorbent to remove heavy metals, nitrate, PO4 and F , (Kalkan et al., 2006 [36]), (f) recovery of Fe, Al, Ti and some other trace metals (Pradhan et al., 1999), (g) treatment acid draining from mines, (Tuazon et.al., 2008 [22], Li Y., 2018 [28]), (h) as geo-tech material to stabilize soil (Deelwal K. et al., 2014 [37]) and many others.

Red Mud Disposal

Red mud is disposed as dry or semi dry (as slurry) material either by crating lagoon /pond, dry stacking or dry disposal. If the mines are at close proximity it is advantageous to dispose the RM residue to those abandoned ditches of bauxite mine in itsparental atmosphere.The RM slurrymixture is comprised of 65-70% liquid and rest solids. The highly alkaline liquid (pH lying between 10-13) can be up to 2 m with high conc. (5-20 gm/ltr) of (Na_2CO_3) escort per one ton of RM which has impact on the eco-health including human (dermatitis, irritation of eyes etc. (Tabereaux Alten 2019 [38])

Methodology

The experimental observations undertaken during the study are: (a) Identification of chemical constituents available in the ingredients of conventional cement concrete andcompared with normalised red mud by using XRF spectrometer. (b) Normalisation of raw red mud by using sea water (c) Finding the physical properties of the ingredients of concrete and NRM (d)Casting of cubes, beams,and cylinders (after curing for 7days, 14 days and 28days under water) at different proportion of mix with NRM (0%, 10%, 20%, & 30%), lime (5%) and superplasticizer (e) Testing the mechanical strength of the cubes, beams and cylinders for their strength (Compressive, split tensile and flexural) by using the CTM and UTM (Compressive strength Machine and Universal Testing Machine) (f) Analysing the result

Comparison of Chemical Ingredients of Cement and RM

The cement industry is prone to high environmental pollution due to release of GHG gas emission though one among the three widely used building materials. The use of bauxite residue can be considered as a part replacement of the cement in construction industry. So the chemical nomenclature of RM and cement is to be done.To substitute RM with Cement, the chemical ingredients must be approximately same and the % of the constituents must be equal or nearly equal. To explore the chemical symmetry of theircementous contributing constituents, the XRF spectroscopy (University Laboratory) was conducted and the outcomes are in Table 1. There is a great dissimilarity in the chemistry of cement and RM. There is a large gap in constituent calcium. So it needs addition of calcium which can be supplemented by adding either CaO or gypsum to supplement it. The % of constituent's differ country wise location wise and types of mines formation. The varying constituent composition and location the normalisation process diverges.

Normalizing Red Mud

The residue RM from Bayer's process is highly alkaline (pH value 10-13) which is toxic to water, soil, vegetation and biosphere. It is due to addition of caustic potash in some midway procedures (Commination, de-silication and digestion) of abstraction of Alumina from bauxite. It is essential to neutralize the residue red mud for open disposal and reuse to ameliorate the environment. Various processes used for limiting pH<8 are (a) using Sea water (b) Acidification, (c) Carbonation, (d) Geo-sequestration (e), calcification associating carbonation and (f) using flue gas. Among the six processes, Sea water can be considered as the cost effective method and sea water act as an adsorbent and reduces the pH of raw RM in two ways. i.e either directly dumping raw RM in sea if the plant is adjacent to coast or transporting sea water to the plant and neutralise the red mud to the required pH value (Rai Sucheta et al, 2012[39] and Tabereaux Alten 2019[38]).

The pH value of residue red mud from Lanjipalli Vedanta plant at Kora put was found to be average 10.8. So the present study uses sea water (BoB at Puri coast) for normalisation of alkaline RM and to find the physical and different strengths (mechanical) of concrete. The red mud powder was first mixed with sea water and kept for 30

minutes and then the slurry was mixed with dry ingredients of concrete and the cubes, cylinder and beams are casted and cured for testing. The sea water + red mud slurry was tested for the pH value and was found to be 8.7 and benign for concrete mix. Practically the salinity remains high due to high Na+ content and need subsequent leaching either by Ca++ ions (Lime or gypsum etc.) are needed, (Hanahan C et al, 2004[40], Rai Sucheta et al., 2013 [39]). To overcome the problem in the present study quicklime was added to reduce the conc. of Na^+ ion in the concrete. But the Vedanta Alumina industry is reducing caustic soda (NaOH) consumption by 10-15 kg/MT of alumina; to minimizedisposal spaceconstraint by 50-60% as they have installed a dry red mud powder plant. They have reduced the quantity of wet red mud storage and have eliminated ecological hazards, http://redmud.org/vedanta-commissions-red-mud-powder-plant-in-odisha

Physical Analysis of RM and OPC

The physical properties of ingredients of cement concrete (IS: 12269-1987) and the blending materials with super plasticizer had been collected and the physical properties like specific gravity (Sp. Gr.), Fineness modulus (FM), soundness, initial and final setting for cement (IS: 8112–1989) water absorption and moisture content for fine (Sand zone III) and Coarse aggregate (HG chips) (Is-383-2016 (R) and the results are in Table 2

Water and Sea water

Sea water was collectedfrom PURI sea beach. The analysis of sea water was carried at CUTM in chemistry laboratory, Jatni. The pH value of sea water is found to be 8.04. The sea water of about 10liters and 20Kg of red mud was made slurry before 30 minutes of making the Normalised Red Mud cement concrete (NRMCC). The normal water from the university taps were used in preparation of normalisedred mud cements concrete NRMCC) with 40% water cement ratio ate a room temperature ranging 28°C-35°C. The pH value of normal water is found to be 7.2.

Super Plasticizer

Dr. Fixity plasticizer was used in the experimental studies. The plasticiser isespeciallymanufactured and used as waterproofing compound and surfactant plasticising polymers and additives. It made the concrete cohesive and prevents segregation. The traditional calculation of design mix was made for M40 grade CC, having targeted design strength after 28days curative adaptation (water) as per IS 10262-2000 (clause 3.2 page -1) was found to be 1: 2.2: 2.9. The % of NRM quantity was varied added are0%, 10%, 20%, and 30% by weight of cement and the casting of specimen was done. The testing sample are 36 no of cubes (150X150X150)mm, 36 no of cylinders (150X300)mm& 36 no of beams (100x100x500)mm (IS 10086 : 1982 and IS 516-1959) ware casted iron mould. The specimens were scientifically placed in curing water tanks after 24 hours of casting for 7,14& 28 days respectively. Present mix proportions adopted in preparation of M40 concrete of cement (Ultra Tech) = 374 kg/cum, NRM =37 kg/cum, water =152 lit/cum, fine aggregate (aggt.) 855 kg/m3&coarse aggregate = 1087 kg/m3, chemical admixture = 8kg /m3 & W/C ratio =0.36.Where the mix design ratio was cement: fine aggt: coarse aggt. = 374:855: 1087=1:2.2: 2.9 and CaO (Hydrated lime) @ 5% by weight of cement and varying wt. of NRM.

Compressive Strength

Compressive (Comp.) strength for cement concrete (CC) of the blocks were established by Comp.Testing Machine (CTM) and Universal testing machine (UTM) as per the specification with 7, 14 and 28 days of curing (IS : 516-1959: 6, table-3)is given **(Table 3 and Fig 2)** as: compressive strength ≥fck+0.825 recognised S.D. approximate up to 0.5 $N/mm^2$and av. comp. strength (fc) = P/A, Where, P= applied load in N and A= cross sectional (CS) area in mm^2
The representative strength should be lower in value than the design. According to standard practice the standard days for finding comp strength are 7th days, 14 days & 28 days should be 65%, 90% & 99 % respectively.

Split Tensile Strength

The tensile strength of CC represents the load at when the concrete member cracks. The cylinders (150 mm □ x 300 mm) were casted and cured for required days. The observational outcomes are given in Table 4 and Fig 3

The formulae used is Split tensile strength = 2p/□dl ; Where, P= maximum applied load in Newton; L=length of the sample in mm; d= diameter (□) of the Sample in mm

Flexural Strength

The beam of size 275mmx75mmx75mm is casted taking bajri as coarse aggregate, river sand &OPC cement and red mud at different percentage such that 10%, 20% & 30%. The suggested breaking load for pedestrian paths allowed is 2KN and residential drive ways is 3KN. Different beams are casted with various % of red mud substation of cement and the breaking load is obtained using UTM after 7days, 14 days & 28 days curing **Table 5 and Fig 4.** The flexural strength (F) =PL/BD^2; where P= maximum load in N; L=span of the length (mm); B= width of the specimen in mm; D = depth of the specimen in mm

RESULTS AND DISCUSSION

The literature survey reveals that the bauxite residue disposed from Bayer's process is highly alkaline and contain concerted iron and titanium oxides and other toxic elements which can deteriorate the soil water and the vegetation of the area. The RM excreted cannot be reused until their high pH > 10 to be reduced to a value pH < 8 for which the slurry need to be normalised. Further researches reveal that normalisation can be done by using Sea water (b) Acidification, (c) Carbonation, (d) Geo-sequestration, (e) calcification etc. but the use of sea saline water is the cheapest method. Further the normalised red mud is deficient of calcium oxide when compared with cement whose manufacturing process evolves huge GHG gasses and polluting the atmosphere. To improve the cementous property of red mud in NRMCC; trials are made by adding NRM with lime or Gypsum. The cost efficient present study involves use of sea water and lime in addition to red mud and experimented at measure strength as cement concrete. Since sea saline water is a good normaliser for the bauxite residue waste; the NRMCC can have better prospective in coastal and under water constructions.

The observations has shown that upto 5% addition of hydrated lime and red mud, the concrete increases its slump value and the workability, making it self-compacting concrete (SCC).The comp. strength gradually increasing for M40 concrete grade after 28 days curing were 45.85N/mm^2 (Orthodox mix),. For blending with 10% NRM + 5% CaO, 20% NRM + 5% Cao and 30% NRM +5% CaO have yielded strength after 28 days curing were 46.75KN/mm^2, 48.35 KN/mm^2 and 44.20 KN/mm^2 respectively. It indicates that beyond 20% NRM substitute the strength id degrading.
The optimum value of split tensile strength is gradually increasing without and with RM at 0%, 10%, 20% and 30% substituting cement (all with addition of 5%lime with RM) and was 5.24Kn/mm^2, 5.33KN/mm^2, 5.85KN/mm^2 and 4.64 KN/mm^2 respectively. Similarly the optimum value of split tensile strength is gradually increasing without and with RM at 0%, 10%, 20% and 30% substituting cement (all with addition of 5%lime with RM) were 6.58KN/mm^2, 6.65Kn/mm^2, 6.80Kn/mm^2 and 5.35KN/mm^2.

The above results infer that the economy % of blending the cement concrete with red mud do not affect the cementous properties along with increasing the mechanical strength and final setting time of NRMCC. The red mud (20%) with hydrated lime (5%) when replace cement do not affect the cement quality or any pozzolanic activity but rather make it self-compacting due to light weight. This enhances the feasibility of substituting cement by 20% NRM and 5% CaO at the optimum. Also it is observed that initially there is affinity of NRMCC for water with increased % of red mud is finer and light in weight. This drawback was removed by using supper plasticizer. The rate of gaining strength increases with time even after 28days curing it further increasing which may be due to low permeability of the NRMCC.

CONCLUSION

It is observed that the percentage of optimum normalised red mud substituting cement is observed as20%. In comparison to other blending materials as substitute of cement like GGBS, Glass dust (from literature), Red mud increases strength at a lower rate but it provide the advantage to maintain a sustainable environment, good soil and good ground water in and around the Bauxite industrial area.Replacement of NRM for Cement is possible from compressive, tensile and flexural strength point of view but need to be verified by exhausts experimental studies. Research is required to address the issue like, corrosion, durability of cement product along with red mud.

REFERENCES

1. Samal, S., Roy, A. K., Bandopadhayay, A., (2013), Proposal for Resources, Utilization and Processes of Red Mud in India — A Review; *International Journal of Mineral Processing* 118:43–55; DOI: 10.1016/j.minpro.2012.11.001
2. Nayak, S., Mishra, S. P., (2016), Nayak, S., Mishra, S. P., Panda, S., (2017), Red Mud the cutting edge of self-compacting concrete, *INPRESSCO, International Journal of Current Engineering and Technology*; 7(2), 390 -396
3. Sing, J., (2019), Effect of red mud as cement replacement on the properties of concrete, International Journal of Innovations in Engineering and Technology (IJIET); 61-66; http://dx.doi.org/10.21172/ijiet.151.08
4. Ruyters, S., Mertens, E., Vassilieva, I., Dehandschutter, B., Poffijn, A., Smolders, E., (2011), The Red Mud Accident in Ajka (Hungary): Plant Toxicity and Trace Metal Bioavailability in Red Mud Contaminated Soil; Environ. Sci. Technology;45 (4), 1616-1622; https://doi.org/10.1021/es104000m
5. Milačič, R., Zuliani, T., Ščančar, J., (2012), Environmental impact of toxic elements in red mud studied by fractionation andspeciation procedures, Elsivier, Science of the Total Environment; 426;359–365; doi:10.1016/j.scitotenv.2012.03.080
6. Mayes, W. M., Burke, T., Gomes, H. I., Anton, A. D., Molnar, M., Feigl, V., Ujaczki, E., (2016), Advances in Understanding Environmental Risks of Red Mud After the Ajka Spill; Hungary, Springer, J. Sustain. Metall; 1-12; DOI 10.1007/s40831-016-0050-z;
7. Pontius, W., (2018), Environmental and Radiation Concerns of Red Mud, *StanfordUniv.*
8. Rathod, R. R., Suryawanshi, N. T., , Memade, P. D.,(2012), Evaluation of the properties of Red Mud Concrete, *IOSR Jr. of Mechanical and Civil Engineering (IOSR-JMCE),* PP: 31-34
9. Sawant, R. A. B., Kumthekar, M. B., Diwan, V. V., Hiraskar, K. G., (2012), Experimental Study on Partial Replacement of Cement by Neutralized Red Mud in Concrete , *Int.Jr. of Eng and Advanced Tech. (IJEAT); 2(1); 2012; 282-286*
10. Sawant, A.B, Kumtheka, M.B, Sawant, S.G, (2013)—Utilization of Neutralized Red Mud (Industrial Waste) inConcrete‖ Inter. Jr. of Inventive Eng.and Sciences (IJIES);1;(9-13), 2013
11. Metilda, D. L. Selvamony, C., Ananda, ku. R., Seeni A., (2015), Investigations on optimum possibility of replacing cement partially by red mud in concrete ,. *Academic journals;* 10(4); 137-143.
12. Sarode, D., Deshmukh, M. P., Pendhari, S. S., Alam, I., (2015), PartialReplacement of Cement in Mortar with Red Mud and Ultra fines,Conf: 2nd R N Raikar Memorial Int. Conf. andBantia- Basheer *Int. Symp. on Adv. in Sc. & Tech. of Concrete; At: Mumbai*, India;II,ISBN No 81-86876-16-2
13. Gowsalya. R, Bhagya, L. A, 2015, Experimental Study on Partial Replacement of Cement by Red Mud, *Int. Jr of Eng Research&Tech. (IJERT),* ISSN: 2278-0181; 3(4), 1-4
14. Deepika, K., Anantha, ku. S., Mariadoss, R, Nanthagopal, J., Saravana, ku. V., (2017),Experimental Investigation of Concrete by Red Mud as Replacement of Cement and Using Strengthening Admixture, *Int. Jr.of Innovative Research in Science*; 6 (3); 3928-3933, DOI:10.15680/IJIRSET.2017.0603164
15. Varghese, M., (2017), Partial Replacement of Cement using Red Mud in SCC, *Int. Jr. of Innovative Research in Sc., Eng. and Technology*, 6 (5), 8333-8338, http:/ /www.ijirset.com/upload/2017/may/175_Partial.pdf

16. Das Mohapatra, P., Mishra, S. P., Nayak, S., Siddique, M., (2019), Optimized Structural Performance of Paver Blocks of Bajri Concrete: NRM Partly Substituting Cement, International Journal of Innovative Technology and Exploring Engineering (IJITEE) ISSN: 2278-3075, Volume-9 Issue-1, November 2019, PP- 1938-49.
17. Menhosh., A, A., Wang Yu, Wang, J., (2017), An Experimental Study of High-Performance Concrete using Metakaolin Additive and Polymer Admixture, Ph.D thesis, University of Salford Manchester; 1-233.
18. Kulkarni, S., (2018), Experimental Study on Red Mud, Fly Ash and GGBFS based Geopolymer Concrete, A Green Substitute to Conventional Concrete, International Journal of Engineering Research & Technology (IJERT); 7 (2); 107-111
19. Das M., Nayak S., Mishra S. P. and Siddique M., 2020, Paradigm Shift on Environmental Sustainability by Replacing GGBS in RMC: Industrial Waste Utilization, *Adalya Journal,* ISSN NO: 1301-2746,;9(3), 970-983
20. Bishetti, P. N., Pamma,r L., (2014), Experimental study on utilization of industrial aste in concrete;*Int. Jr.of Technical Research and Applications*, 2(4), 49-52.
21. Pujar, S. M., Prakash, K.B., (2014), Effect of Replacement of Cement byRed mud on the Properties of Concrete, *Int. Jr of Sc. & Eng. Research*; 5 (9); 805-814
22. Tuazon, D., Corder, G. D., (2008), Life cycle assessment of seawater neutralised red mud for treatment of acid mine drainage, *Resources, Conservation and Recycling*, Vol. 52, pp. 1307–1314, DOI: 10.1016/j.resconrec.2008.07.010
23. Snigdha, S., Batra, V. S., (2008), Catalytic applications of red mud, an aluminium industry waste: A review, *Elsevier, Applied Catalysis B Environ*; 81(1–2); 64-77,
24. Riberio, D. V., Labrincha, J. A., Morelli, M. R., (2012), Effect of red mud addition on the corrosion parameters of reinforced concrete evaluated by electrochemical methods; *Cement and Conc. Research;* 42(1):124–133; DOI: 10.1016/j.cemconres. 2011.09.002
25. Tauber, T., Hill, R. K., Crook, D. N., Murray, M. J., (1971), Red mud residues from alumina production as a raw material for heavy clay products, *J. Austr. Cera. Soc.*; 7 (1); 12-17
26. Satapathy, B. K., Patnaik, S. C., Vidyasagar, P., (1991), Utilisation of red mud for making red oxide paint, INCAL-91, Int. *Conf. and Exhibition on Aluminium at Bangalore, India 31st July-2nd,* (1): 159-161.
27. Garg, A., Yadav, H., (2015), Study of Red Mud as an Alternative Building Material for interlocking Block Manufacturing in Construction Industry, *International Journal of Materials Science and Engineering*; 3 (4); 295-300 .
28. Lima, M. S. S., Thives, L. P., Haritonovs, V., Bajars, K., (2017), Red mud application in construction industry: review of benefits and possibilities, *IOP Conf. Ser.: Mater. Sci. Eng.*; 251; 1-10, doi:10.1088/1757-899X/251/1/012033
29. Li, Y., Li, W., Xiao, Q., Song, S., Naidu, R., et al., (2018), Acid mine drainage remediation strategies: A review on migration and source controls, *Springer-Mining, Metallurgy & Exploration*; 35, 148–158, https://doi.org/10.19150/mmp.8464
30. Liu, Dong-Yan,and WuChuan-Sheng, (2012), Stockpiling and comprehensive utilization of Red Mud, Research Progress, *Materials;* 5; 1232-1246; doi:10.3390/ma5071232
31. Amritphale, S. S., Anshul, A., Chandra, N., Ramakrishnan, N., (2007), A novel process for making radiopaque materials using bauxite-Red mud. *Journa of the European Ceramic Society*; (27):1945–1951.
32. Pontikes,,Y., Nikolopoulos, P., Angelopoulos, G. N., (2007), Thermal behavior of clay mixtures with bauxite residue for the production of heavy-clay ceramics. *Journal of the European Ceramic Society*; (27):1645–1649.
33. Arhin, D. D., Konadu, D. S., Annan, E., Buabeng, F. P, Yaya, A., Tuffour, B. A., (2013), Fabrication and Characterisation of Ghanaian Bauxite Red Mud-Clay Composite Bricks for Construction Applications, *American Journal of Materials Science;* 3(5): 110-119.
34. Busto, R. V., Gonçalves, M., Coelho, L. H., (2016), Assessment of the use of red mud as a catalyst for photo degradation of bisphenol: A in wastewater treatment, Pubmed, *Water SciTechnol*; 74(6); 1283-1295
35. Velumani, P., Senthil, Ku. S., (2017), Production of sludge incorporated paver blocks for efficient waste management, *Taylor and Francis, Journal of the Air & Waste Management*, DOI:10.1080/10962247.2017.1395373:
36. Batham, G., (2018), Strength enhancement of paver block using red mud, *International Research Journal of Engineering and Technology, (IRJET);* 05(7) ; 585-589
37. Kalkan, E., (2006) Utilization of red mud as a stabilization material for the preparation of clayliners; *Engineering Geology*; (87):220–229.

38. Deelwal, K., Dharavath, K., Kulshreshtha, M., (2014), Evaluation of characteristic properties of red mud for possible use as a geotechnical material in civil construction, *Int. Jr. of Advances in Eng. & Tech*; Vol-7(3), PP-1053-59.
39. Tabereaux, Alton, (2019), Addressing the Challenge of Bauxite Residue; https://www.lightmetalage.com/news/industry-news/smelting/article-addressing-the-challenge-of-bauxite-residue/
40. Rai, Suchita.,Wasewar, K. L., Mukhopadhyay, J., Yoo, C. K., Uslu, H., (2012), Neutralization and utilization of red mud for its better waste management, *ARCH. ENVIRON. SCI.*; 6, 13-33
41. Hanahan, C, McConchie, D., Pohl, J., Creelman, R., et al., (2004), Chemistry of sea water neutralization of bauxite refining residues (red mud), *Env. Eng. Science*; 21: 125–138; https://doi.org/10.1089/109287504773087309
42. Tharani, P., Adithiya, B. A., Murali, K., (2017), Experimental Study on Concrete with Bauxite Residue as Partial Replacement of Cement, *International Journal of Chem Tech Research*, vol. 10, pp. 35-41, 2017.
43. Tang, W. C., Wang, Z., Liu, Y., Ciu, H. Z., (2018), Influence of red mud on fresh and hardened properties of self-compacting concrete, Construction and Building Materials, vol. 178, pp. 288-300, 2018.

Table 1: The assessment of chemical ingredients between cement and normalised Red mud

Cementous Oxides	Formulae/ Unit	Bauxite residue Moise et al. 2017	Cement	NRM	Impairing properties	If Excess
Calcium	CaO (%)	5-23	63	3.96	Strength	expand & disintegrate
Silicon	SiO_2 (%)	0.8-2.3	22	11.53	Strength	Extend setting time
Aluminium	Al_2O_3 (%)	10-22	6	14.14	Early set	Weaken cement
Iron	Fe_2O_3 (%)	31-43	3.35	42.52	Colour	alter impart strength
Sodium	Na_2O (%)	3-5	Nil	8.85	Alkaline	alkali-aggt reaction, efflorescence / staining
Magnesium	MgO (%)	0.3-0.7	2.5	0.05	Hardness	Colour
Water	H_2O	H			Hydration	affect workability
Sulphate	SO_3^{--}	S			soundness	early setting

Source: http://www.engineer ingenotes.com/concrete-technology/cement-concrete-technology /cement-characteristics-properties- composition-harmful-constituents-and-uses-engineering-materials/46449

Table 2: The physical characteristics of the Cement, Sand and Chips and the NRM used

Physical Quantity	Unit	Cement	NRM	Sand Zone III	Chips	Apparatus	IS Code followed
Product used	Ultra Tech						
Specific Gravity	Sp Gr.	3.2	2.7	2.74	2.85	Sp. Gr. bottle	IS: 4031 (2)–2005
Fineness Modulus	Sieving	3%	4.0%	2.7	0.8	Sieve analysis	IS 4031-(1)-1996
Consistency	32 % H_2O	8mm	-	-	-	Vicatapprat us	IS: 4031 (4) – 1999
Soundness	in mm	5mm	-	-	-	Li-Chat appar.	
Initial setting Tine	Min	35	-	-	-	Vicat'sappar.	IS: 4031 (5) – 1999
Final Setting Time	Min	586	-	-	-	Vicat'sappar.	IS: 4031 (5) – 1999

Grain size distrib^{n}	n = D60/D10)	-	Clay	Zone III	-	Sieve analysis	IS: 2386(-1) – 2016
Moisture content	%		10.35%	1.2%	1%	-	-
Bulk density	gm/cm^3		2.13			-	--
Water absorption				1%	0.4%	-	-

Source: For sand and HG chips the IS codes referred are Is-383-2016(R), IS 15658 (2006) for Red mud: Tharani P. et. al., 2017 [41], Tang W. C. 2018[42], Feng B & Wang 2018 [43],

Table 3:The compressive strength of cubes of NRMCC at various % with NRM and Lime

CC with %NRM & Lime	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2	N/ mm^2
Test	Step - 1	Step - 2	Step - 3	Avg.	Step - 1	Step - 2	Step - 3	Avg.	Step - 1	Step - 2	Step - 3	Avg.
M40 CC	30.1	31.5	32	31.20	41.45	43.02	43.95	42.80	46	45.5	46.35	45.85
10%NRM ,5% CaO	32	33.35	33.5	32.95	44	43.58	42.02	43.20	46.43	45.35	48.18	46.75
20%NRM, 5% CaO	32.96	35.23	35.61	34.60	45.59	44.81	44.45	44.95	47.14	48.79	49.12	48.35
30%NRM, 5% CaO	32.12	31.98	30.85	31.65	41.27	41.53	39.75	40.85	44.96	45.14	42.65	44.20

Table 4: The split Tensile strength of cylinders of NRMCC at various % with NRM and Lime

% substitute	7 days comp. strength (N/mm^2)				14 days comp. strength(N/mm^2)				28 days comp. strength(N/mm^2)			
Test	S-1	S-2	S-3	Avg.	S-1	S-2	S-3	Avg.	S-1	S-2	S-3	Avg.
M40 CC	4.1	4.51	5.0	4.54	4.53	4.69	5.36	4.86	4.95	5.0	5.77	5.24
10% NRM , CaO 5%	4.2	4.68	5.2	4.69	4.54	4.72	5.65	5.1	5.1	5.15	5.74	5.33
20%NRM , CaO 5%	4.35	4.96	5.35	4.88	4.62	4.86	5.88	5.24	4.94	5.28	5.35	5.85
30%NRM , CaO 5%	4.0	4.19	4.26	4.15	4.12	4.16	4.56	4.28	4.1	4.82	5.0	4.64

Table 5: Flexural strength of beamsof NRMCC at various % with NRM and Lime (Comp. Strength is in N/mm²)

% substitute	Comp. strength 7 days (N/mm²)				Comp. strength14 days (N/mm²)				Comp. strength28 days (N/mm²)			
Test	S-1	S-2	S-3	Avg.	S-1	S-2	S-3	Avg.	S-1	S-2	S-3	Avg.
M40 CC	5.48	5.45	5.47	5.46	5.92	5.98	5.97	5.95	6.55	6.61	6.58	6.58
NRM 10% , CaO 5%	6.2	5.9	5.0	5.70	5.98	5.97	6.01	6.1	6.32	6.70	6.61	6.65
NRM 20% ,CaO 5%	6.4	5.93	5.77	5.92	6.8	6.0	6.3	6.37	6.42	6.85	6.92	6.80
NRM 30% ,CaO 5%	5.0	4.9	4.7	4.85	5.12	5.05	4.56	4.89	4.3	5.75	6.0	5.35

Fig 1: Bauxite residue, the test samples, the lab work, The CTM & the XRF spectrometry

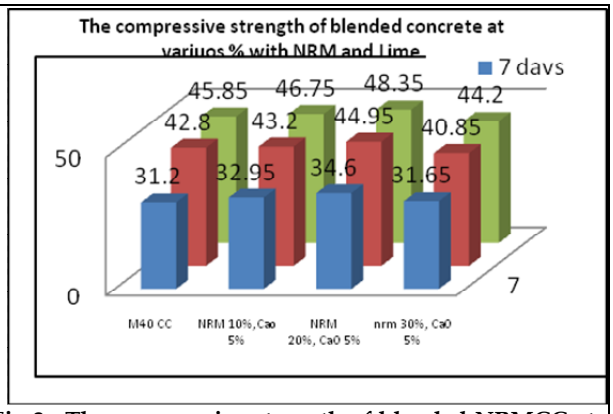

Fig 2 : The compressive strength of blended NRMCC at various % with NRM and Lime

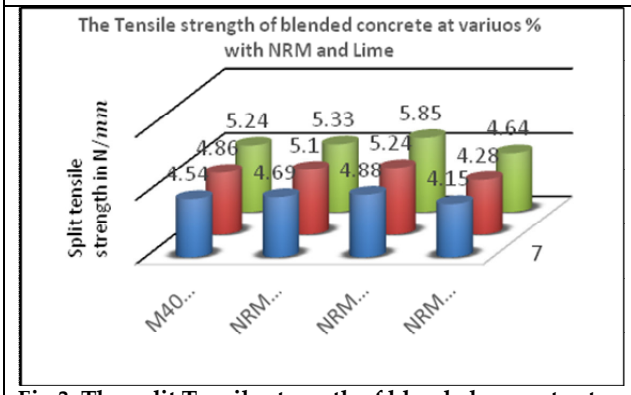

Fig 3: The split Tensile strength of blended concrete at variuos % with NRM and Lime

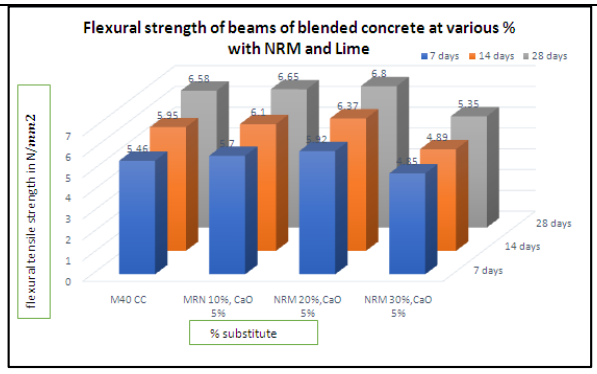

Fig. 4: Flexural strength of beams of blended concrete at various % with NRM and Lime

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RESEARCH ARTICLE

Part Substitute of River Sand by Ferro chromes lag in Cement Concrete: Industrial Waste Disposal

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ABSTRACT

Slags obtained from Ferrochrome (FeCr) plants are industrial wastes left to nature which pollutes the soil and water making the surrounding barren and deprived of vegetation. To sustain the environment the research intends to replace the FeCr slag as coarse or fine aggregate substitute. The slag generated during manufacture of FeCr alloy whichis a stable, dense, crystalline product having tremendous thermal, mechanical and engineering properties found suitable forpartial substitute as fine aggregate material (sand) in concrete. Present studyenvisages replacement ofFeCr slag with conventional fine aggregate in concrete for achieving high strength(M40Grade) concrete for every incremental of 20% replacement up to 100% is investigated.The hardened properties of concrete is determined by casting test cubes for compressive strength, cylinders for split tensile strength and prisms for flexural strength for 7days, 14days and28days curing. The results are compared with conventional fine aggregate and the corresponding physical and mechanical properties for M40grade concrete verified at different mixes. The results exhibits that 60-80%replacement of FeCr slag against normal river sand in cement concreteis the optimum substitution considering compressive strength. This shall add to safe disposal of Fero-chrome ally plants in hilly, coastal and muddy areas where suitable river sand is not available and coastal areas

Keywords: Ferrochrome Slag, Fine Aggregate, Mechanical strength, natural sand, UTM, XRF spectrometry

INTRODUCTION

Concrete is a versatile material widely used as principle element for structures and for other applications. The demand on concrete is increasing day by day due to the growing population, housing, transportation and other amenities. As a result the demand for concrete making materials also increases leading to the scarcity of naturally

available fine and coarse aggregate required for concrete making. Additionally, the fast industrialization hascontributed to different types of wastes as residues or by-products which is environmentally toxic and creates problem in disposal. Hence, utilization of suitable waste bi-products or reused activities of the environment degrading waste is essential.

Construction industries have become an inevitable option in recent days by fulfilling the demands of concrete as well as reduction in impact on environment. The use of industrial waste as aggregates in concrete provides good platform to utilize the waste as alternatives to naturally available aggregates in concrete as aggregates are the main constituents of concrete making about 75% of its total volume. Ferrochrome (FeCr) slag (Fig 1) is one of the alternative materialswhich can be used as both coarse and fine aggregate for replacement of river sand andcrushed rock ballast in concrete by altering the physical formlike thermal conductivity and specific heat (Al-jabri et al 2018[1]).

FeCr Slag

Ferrochrome slag a waste by-product generated during the manufacturing of Ferrochrome alloy. Ferrochrome alloy ismanufactured in a submerged electric arc furnace by physio chemical process at thetemperature of 1700^0C. Individually the molten liquids of the ferrochromium and slag flowout into dippers. Due to the different specific gravities of metal and slag, separation of thetwo liquids takes place. The liquefied ferrochrome slag gradually cools down in air (air cooled) forming stable, dense, crystalline product having tremendous mechanical properties. The FeCr slag contain chemical ingredients in dry process such as Al_2O_3 (22-30%), SiO2 (26-29%), MgO (23-30.5), CaO (2-3%), Cr_2O_3 (≈ 8%), FeO (≈ 3-4%).The typical ferrochrome slag which is basic and pH value is about 8. (Panda et al 2013[2],Kopuri et al 2017[3])whereas water cooled FeCr residue has more Cr_2O_3 (>10%) which is more harmful and toxic (Laxmipriya et al., 2018[4]).The heavy noxious metals like Zn, Cd, Hg, As and Pb are available in trace (Urs N et al., 2018[5]) The cement concrete prepared by FeCr slag sand imparts diverse characteristics like leaching, micro-structural and mechanical properties. However the fine particle of FeCr obtained from the alloy plant is tested by X-ray Fluorescent spectroscopy,(Epsilon 1 PAN analytical B. V., the Netherlands make)of in the University Laboratory and the chemical constituents are in Table 1:

The reuse of Ferrochrome slag is limited when associated to its generation. They are mostly used in civil engineering constructions and pavement structures and filling works. The use of ferrochrome slag can reduces the procurement of natural aggregates and reduces the impact on environment. Although the waste slag has excellent properties, its usage has been limited due to its potentiality of discharging dangerous chromium compounds to the environment. In the present study, Ferrochrome Slag Sand is assessed for its suitability to partially and fully replace the fine aggregate in M40 Grade concrete.

LITERATURE REVIEW

The generation of FeCr slag is 6.5 to 9.5MMT/year and is increasing @2.8 to 3 % per annum (Kauppi and Peka, 2007[6]). Ferrochrome residue is still land filled due to chromium as constitutent and environmental issues (Holappa et al., 2004[7], Horkmans et al., 2019[8]). The FeCr slag obtained from Ferrochrome alloy plants in particle size can replace the river sand used as fine aggregate in high strength cement concrete (Panda et al., 2013[2], Somyashree et al., 2017[9], Dash M. K. et al 2018[10], Laxmi Priyaet al. 2018[4], Kopuri et al., 2019[3]). The residual chromium in FS as Cr (III) remains immobilized in the stable spinal phase like magnesium aluminum chromates $Al_2(CrO_4)_3$, magnesium chromate (Mg CrO_4), which inhibit the release of chromium from the slag matrix under ambient environmental condition and Cr^{++} ion is toxic for the ecosystem and water portability Panda et al. (2013)[2].

FeCr slag products is in use as filling construction materials,sub surface drainage and replacing natural sand and macadam in Finland from 1970's since low leaching properties, (Niemelaet al., 2007[11]). The feasibility of partial replacement of cement by the FeCr dust and lime is under study and the problems isworkability, consistency and

setting time, (Acharyaet al., 2015[12]). The replacement of ferrochrome slag with conventional coarse aggregate in concrete for M25 grade and even high strength (M50 Grade) concrete for every incremental of 25%replacement up to 100% can be possible (Susheel et al., 2016 [13] and Sathwik et al., 2016[14]).

Experimental Programme

Material Properties

The materials required for the tests are grade 53 OPC, river sand, Black hard granite chips, FeCr fine particles, water and super plasticizer **(**Fig 2**)**

Cement

The products used in this investigation are of grade 53 Ordinary Portland cement (OPC) with a specific gravity (Sp. Gr.) of 3.20 with 34 and 505 minutes for initial and final setting time's respectively.

Coarse Aggregates

Black hard granite rock Ballast (Machine crushed) as Coarse aggregate is obtained from a local quarry. The Coarse aggregate is confirming to grading zone-IV of table-1 of IS: 383.Typical Properties of Maximum nominal size of aggregate 20mm,Coarse aggregate Specify gravity 2.65, Water absorption of 12 -20mm chips (coarse aggregate) is 1.5.

Fine Aggregates

The Fine aggregate used is naturally available river sand in the nearby Dayariver. The properties of Fine aggregate are determined from experimental investigations and presented in Fine aggregate is confirming to IS 2386-3 (1963). The physical properties of the medium quality sand used are of Specific gravity 2.69, fineness modulus 3.31, water absorption 1.8, loose bulk density 1.62 and the particle size distribution is of Zone III IV (IS 373-2016).

Ferrochrome Slag Sand

Ferrochrome slag aggregate used in this study, is a waste material collected from a dump yard at M/S.Stork Ferro and Mineral Industries Pvt. Ltd ,RemunaBalasorein Odisha .The Ferrochrome slag sand properties are Specify gravity of ferrochrome slag sand 2.82, Water absorption of1.9,Fineness of Ferrochrome slag sand 3.83 and pH 7.34 .

Super Plasticizer

Sika super plasticizer is used as a cement additive in concrete due to its pozzolanic nature. Sika increases the workability and strength of concrete. . It makes concrete cohesive and prevents segregation.

Mix Design and Mix Proportion

The laboratory works such as physico- mechanical properties of the ingredients of the present study has been conducted in the Centurion University Technology and management laboratory, Jatnithe physical properties of the ingredients were identified according to the available standard laboratory processes. The targeted compressive strength (Comp. Strength) was found using IS 456-2000.The mix is designed to have a minimum slump of 25-50mm. It is observed that the cement content required for mix proportioning exceeds the design stipulations hence Sika super plasticizer is replaced with weight of cement. The formula used is $fck.' = fck. + 1.65s.$ From Table I of IS10262 :2009 Standard Deviation ,S=5N/MM² ,Therefore target Strength = 40 +1.65s =48.25N/mm².The % of addition of Ferrochrome slag sand varied from 0%, ,20%, and 30% 40% ,60%,80%,100% by weight of the cement and the specimen was casted .Applying standard procedure of calculation as per IS 456-2000, the quantity of ingredients calculated are cement =427kg/m3, water = 154 ltr /m3, the fine aggregate=701kg /m3, coarse aggregate-973kg\m3, Chemical admixture=8kg/m3 under W/C ratio=0.36. The final design mix proportion by weight was found to be

1:1.64:2.27. Cubes, cylinders and beam werecasted and cured by portable supply water of CUTM for 7, 14 and 28days for different mix proportions and replacements

RESULTS AND DISCUSSION

This chapter deals with the presentation of test result, and discussion on compressive strength development of ordinary concrete. The test result of various tests performed on fresh concrete and Fine aggregate with replacement of Ferrochrome Slag as Sand at different percentages are presented in the tables below and the casting and testing processes are in Fig 3.

Compressive Strength

Compressive strength of concrete tells about the strength the concrete can withstand compressive load. From different substitute of FeCr Sand replacing natural fine aggregate (sand) shows there is a regular increase and at 60%, 80% and 100% substitute the loading capacity is 40.95, 43.8 and 48.29 N/mm2. Fig 4 and Table 2

Split Tensile Strength

The tensile stress (Split: SPTS) an indirect method of tensile strength testing of concrete at acts evenly on the line of action of load as per IS 5816: 1999. The formula used is T= 0.637P/dl Where, T = SPT in MPa P = Functional load, D = Dia. of the sample CC Concrete cylinder. The optimum results obtained after 7. 14, 28days curing are when the FeCr substitute for sand is gradually increasing and optimum at 80% substitute (Fig 5 and Fig 6).

Flexural Strength

According to IS: 516 – 2002, It is the Flexure (toughness) which is imparted to the cement concrete so that it tends to bend the test beam casted from the cement and its ingredients. The flexural strength or the modulus of rupture is the materials ability to resist deformation. The modulus of rupture (F_b) is: $f_b = \frac{Pl}{bd^2}$ when a =line of fracture and the nearer support is>20.0cm for 15.0cm beam sample or > 13.0cm for 10cm sample beam specimen), b = width (cm), d = depth to failure (cm) and l = lengthof support (cm). In the present case the maximum flexural strength is when the FeCr substitute is 80% (6.15 N/mm^2) and and at 60% substitute it is (5.0 N/mm2)**(**Fig 7)

DISCUSSION

Ferrochrome slag is economically available and sustainable.Environmentally the FeCr slag is toxic due to chromium, at a concentration of 1–2 wt % for air cooled slags and 5–10 weight % in water cooled FeCr slag. Many ferrochrome alloy industries have also face the problem regarding the acute disposal of this byproduct. However a noteworthy solution may consist of a proper utilization of these Sand in different construction processes. The materialbehaviour is mostly similar to that of Fine aggregates. So it can be used as a better substitute for Fine aggregates. Moreover the complete elimination of Fine aggregates andthe complete utilization of slag may affect the qualitative as well as quantitative perspectives in different sectors. Hence a hybrid utilization of both Fine aggregates and Ferrochrome slag sand may be convenient for construction purposes. In this project a brief methodology is proposed and the optimum hybrid proportions are identified after the evaluation of materialproperties. The concrete shrinks after 28days curing or hydration process when completes but this property is found to be improved when there is partial substitution of FeCr slag particle with sand (Al-Jabri et al., 2018[1]).

According to the literature review 60-80% utilization of Ferrochrome slag sand giveadequate strength when substituted by normal river sand in orthodox concrete . So various trials are executed (0-100%) and from which the100% use of slag gave greater mechanical strength. However the 60-80% trials are more or less higher than the targeted strength and closer to the higher result. A marginal decrease is observed except in 40 % and 100 % trials. So

to say some environmental factors and curing conditions are there which affects adversely to the compressive strength. Somehow from the research, it can be concluded that 60 - 100 % utilization will be efficient, provided proper curing and environmental exposures should be encountered. Further on exposure of the samples in the drains, sea water and highly diluted HCl solutions have about no impact on the properties like efflorescence, chloride attack to the cubes and extension to the study could not be completed for paucity of time so can be best used in coastal areas.Similarly the ecosphere degrading ferrochrome slag granules can add to safe disposal of Fero-chrome ally residue in hilly, coastal and muddy areas where suitable river sand is not available.

CONCLUSION

Ferrochrome (FeCr) slag is a waste bi-product from Ferro Chrome alloy plant. The chemistry of the FeCr sample for its chemical ingredients have been found for its constituents by XRF Spectrometer. The properties (Physical, Chemical and mechanical) of materialswith the mix design has been done as per IS code standards. The samples (cubes, cylinders and beams) along with laboratory testsare accomplished on green concrete and the workability of concrete is measured in the laboratory. After 7, 14 & 28days water curing, the mechanical properties like comp. strength of cubes, SPTS for cylinders and toughness (modulus of rupture test) for beams are executed by using either CTM or UTM.Present study tells that the Comp. strength, SPTS and the modulus of rupture has optimum values differing ate different % of mix of FeCr granules. The optimum is either reached when the replacement of river sand is done by FeCr between the 60-80%.Ferro chrome slag when replaces with fine aggregate it resistant to acid and base attacks caused by water.

REFERENCES

1. Al-Jabri K., Shoukry H., Khalil I. S., NasirS., 2018, Reuse of Waste Ferrochrome Slag in the Production of Mortar with Improved Thermal and Mechanical Performance, ASCE, Jr. of Materials in Civil Engineering; 30(8);
2. Panda C.R., Mishra, K.K., Panda, K.C., Nayak, B.D., Nayak, B.B.,(2013).“Environmental and technical assessment of ferrochrome slag as concrete aggregate material”. Constr. Build. Mater. 49, 262–271.
3. Kopuri N.A.G.K.M, Ramesh K., 2019, Strength and Durability Studies on Concrete with Ferro Chrome Slag as Partial Replacement to Fine Aggregate, Int. Jr. of Recent Technology and Engineering (IJRTE); 8(1), 754-758
4. Lakshmi Priya P S, Anu V. V., 2018, Use of ferrochrome slag as aggregate in concrete- a review, Int. Research Jr. of Engineering and Technology (IRJET); 5(11); 1500-1506.
5. UrsNeethu, AnwerMd D., 2018, using of ferro-chrome slag as a coarse aggregate and stone dust as a fine aggregate, Int. Research Jr. of Engineering and Technology (IRJET); 5(11); 686-692.
6. Kauppi, M. and Pekka, N., (2007). “Production, characteristics and use of Ferro-chrome slags”, Infacom 7.
7. Holappa, L.; Xiao, Y., 2004,Slags in ferroalloys production—Review of present knowledge, Jr. South Afr. Inst. Min. Metall; 104; 429–438
8. Horckmans L., Möckel O. R., Nielsen P., Kukurugya F., et al.,2019, Multi-Analytical Characterization of Slags to Determine the Chromium Concentration for a Possible Re-Extraction, MDPI, Minerals 2019, 9(10), 646; https://doi.org/10.3390/min9100646
9. Somyashree M. A., 2017, Partial Replacement of Natural Aggregates withFerro-chrome Slag, Int. Jr. for Research in Applied Sc. & Eng. Tech. (IJRASET,), 5(6); 1357-1361
10. Dash, M.K. and Patro, S.K. (2018), “Performance assessment of ferrochrome slag as partial replacement of fine aggregate in concrete”, Eur. J. Environ. Civil Eng., 1-20.https:// doi. org/10.1080/19648189.2018.1539674
11. Niemela P and Kauppi M (2007) “Production, characteristics and use of ferrochrom slags”. In: INFACON XI, New Delhi, India, pp.171–179.
12. Acharya K P, Patro K S,(2016) “Utilization of ferrochrome wastes such as ferrochrome ash and ferrochrome slag in concrete manufacturing”, Waste Management & Research1–11

13. Susheel S M, Sathwik S R, VinayakT,Darshan S, Sanjith J and Ranjith A, (2016)"Development of Normal Strength Concrete using Ferrochrome Slag Aggregate asReplacement to Coarse Aggregate", IJISET – Inter.l J. of Innovative Science, Engineering & Technology, 3 Issue.
14. Sathwik S R, Sanjith J, Sudhakar G N, (2016) "Development of High Strength Concrete Using Ferrochrome Slag Aggregate As Replacement to Coarse Aggregate ", AJER -American Journal of Engineering Research, Volume-5, Issue-9, pp-83-87.
15. Indian standard code of Practice :IS 2386-3 (1963).
16. Indian standard code of Practice : IS 383- (1970 and rev 2016).
17. Indian standard code of Practice : IS 10262- (2009).

Table 1: the chemical compositions of ferrochrome slag

Chemical	Form	Present	Chemical	Formula	Present	Chemical	Formula	Present
Aluminum Oxide	Al_2O_3	22.20%	Chromium Oxide	Cr_2O_3	27.22%	Zirc. Oxide	Zr_2O_3	237ppm
Silicon dioxide	SiO2	32.47%	Manganese Oxide	MnO	0.61%	Tin Oxide	SnO_2	181ppm
Phosphorous Pentoxide	P_2O_5	0.52%	Iron Oxide	Fe2O3	6.98%	Yiterbium Oxide	Yb_2O_3	66ppm
Sulpher Trioxide	SO_3^{--}	1.04%	Nickel oxide	NiO	869ppm	Irridium Oxide	IrO_2	72ppm
Chlorine	Cl	878ppm	Zinc Oxide	ZnO	706ppm	Bismuth Oxide	Bi_2O_3	15ppm
Pot. Oxide	K_2O	0.41%	Selenium Oxide	SeO_2	9.4ppm	Titanium Ox.	TiO_2	0.434%
Calcium Oxide	CaO	7.74%	Stronsium Oxide	SrO	235ppm	Yitrium Oxide	Y_2O_3	29ppm

Table 2:Compressive strength (7, 14, 28 days) of feCr slag cement concrete cubes N/mm²

Sl. No	Percentage of replacement	7days comp. strength	14days comp. strength	28 days comp. strength
1	0	23.48	28.6	35.95
2	20	29.5	34.7	45
3	40	28.25	32.45	41.2
4	60	26.55	35.35	40.95
5	80	20.55	34.1	43.8
6	100	24.55	35.3	48.29

The strength obtained is slightly less than the required comp. strength of M40 C

Fig 1: The fine particles of FeCr slag at Balasore Ferro alloys Ltd, Somona

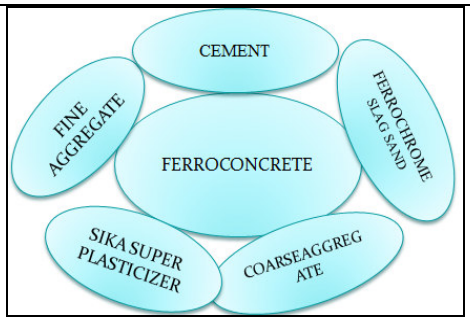


Fig 2: The materials FeCr concrete used for study

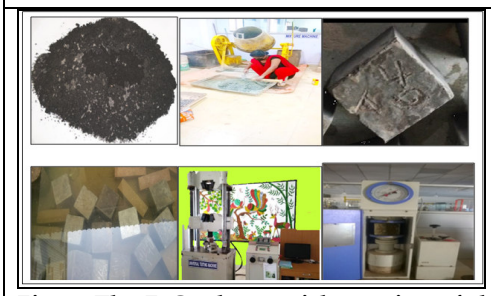


Fig. 3: The FeCr slag particle, casting of the samples, Universal testing machine and CTM

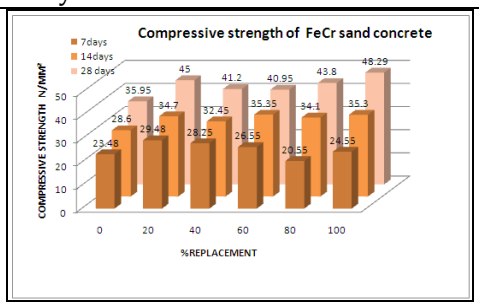
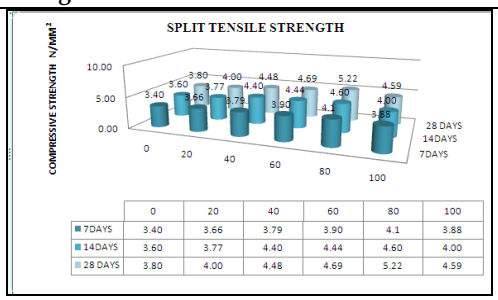


Fig 4: Comp. strength (after 7, 14, 28 days curing) of FeCr slag CC cubes N/mm2

Fig 5: The cylinders after casting after mixing with different % of substitute of FeCr granules



	0	20	40	60	80	100
7DAYS	3.40	3.66	3.79	3.90	4.1	3.88
14DAYS	3.60	3.77	4.40	4.44	4.60	4.00
28 DAYS	3.80	4.00	4.48	4.69	5.22	4.59

Fig 6: Split tensile strength (after 7, 14, 28 days curing) of FeCr slag CC Cylinder N/mm2

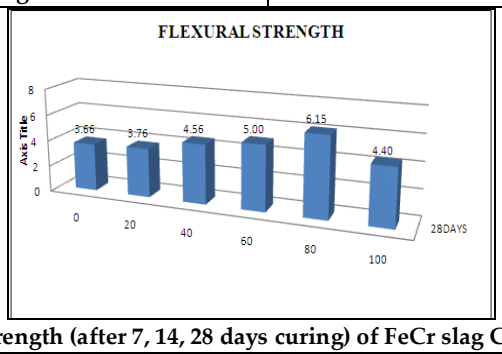


Fig 7: Flexural strength (after 7, 14, 28 days curing) of FeCr slag CC beams N/mm2

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RESEARCH ARTICLE

Study of Diversity of Molluscs from Puri Sea Beach, Odisha, India

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ABSTRACT

Baliharchandi estuary situated in the Puri district at the east of Odisha, which is 27 km to Puri sea beach. This estuary is the connected area of Puri and Chandrabhaga sea beach. An initial study was conducted by me to explore the malcofauna diversity and their morphological study. The duration of study was two months. Studied were conducted by hand picking method, digging substratum, collected species preserved in plastic jar and photographic captured. The study yielded 17 molluscan species belonging to 2 classes, 9 order, 15 family. It was conducted that Baliharchandi is rich in Gastropoda and Bivalvia. 13 species belong to the Gastropoda and 4 species belongs to the Bivalvia were collected. *Cerethidea cingulata*(Gmelin, 1791) was the most abundant molluscan species present and then *Teleoscopium teleoscopium* was the second highest in the estuary

Keywords: Molluscs, Cinguata, Teleoscopium,Puri, Baliharchandi

INTRODUCTION

Molluscs are belongs to the kingdom Animalia which are mostly marine. Mollusca is derived from the word *mollis* which mean soft bodied. They are diverse in nature. Molluscs are most abundant among all marine animals so it acts as an important constituent in the marine diversity. They are highly diverse reference to their size, anatomical structure, behavior and habitats. Due to its abundance it provides vast ecological functions like commercial, social, asthetic and medicinal value (SubaaRao 2003). In modern human society they are an important source of food and also provide a suitable surface for many microbenthic organisms to form colonies over their body (SubbaRao 2003). Mollusca is the second largest phylum after arthropoda. Molluscs are most abundant of all animals. It covers 23% whole marine living animals (Mantosh and JaydevMoity 2018). These are most ancient animal and they appear in the oldest Cambrian deposits, more than 550 million years ago (Haszprunar G &Wanninger A 2012). According to David

Nicol in 1969 the total number of living molluscs species are 107,000 from which 12,000 from fresh water gastropods and 35000 from terrestrial. According to Morton JE in 1958 molluscs are plastic material in an evolutionary sense. Though the fossil record does not explain about all families and genera through time. Many taxonomic levels have appeared, radiated and disappeared over the time period.

In India Asiatic Society of Bengal (1784) initiated about exploration of Mollusca, which was in 18th century. Then in 20th century zoological survey of India significantly works on this exploration of Mollusca. Odisha is one of the maritime states in east Indian coast which have various type of coastal ecosystem, which basically comprises of estuaries, coastal lagoons, creeks, intertidal mudflats, stony and sandy beaches and mangroves swamps contains bearing high molluscs diversity. The state of Odisha having many estuaries i.eChilika, Bhitarkanika, Mahanadi, Dharma, Subarnarekha and many more.Due to the variety of coastal ecosystem comprising estuaries, creeks, coastal lagoons, sandy beaches, swamps having high Mollusc diversity.The Baliharchandi estuary of Puri which lies on eastern coast of the state Odisha. This place is sandy beach and the meeting point of river Bhargavi with the Bay of Bengal. My study is basically focused on to found in some of the selected areas of the Puri district. There have reported some particular species of Mollusca in much in number rather than in variety.

Taxonomic History and Classification

The classification of phylum mollusc took a long change from days of Aristotle to the present. Aristotle (384-322B) broadly classified molluscs into Malachia now it called Cephalopoda and Ostracodermata (the shelled form). In between 23 to79 AD; Malachia was changed to Mollia and Ostracodermata to Testacea by Pliny (the Elder) and finally during the 17th century exactly on 1650 Jonstonus was finally changed ollia to ollusca. The contribution of Linnaeus in 1758, Cuvier in 1795, Dumeril in 1806 and Jean Lamarck from 1801 to 1809 gradually changes the hierarchical structure of molluscs over the consecutive years. (www.biologyeducation.net,2011).

In 1795, Cuvier was published revised classification of Mollusca. In 1825, De Blainvillealter the name Mollusca to Malacozoa, which helps to malacology, malacologist, etc. Larval stages of barnacles and categorized them to be crustaceans was done by J. Thompson and C. Brumeister in 1830. In 1866 A. Kowalevsky removed the tunicates from the Mollusca. Separation of brachiopods from the molluscs was controversial ordeal and that was continue to the end of the 19th century. In the year 1841 Swedish naturalist Loven were discovered Aplacophorans. External characteristics, Anatomical differentiation, Molecular genomic differentiation and structure of protein played an important role in classification of molluscs so the grouping of the gastropoda changed accordingly. According to Richard C Brusca and Gary J Brusca in 2002 explain that there are two subphyla and seven classes of molluscs: Aplacophora, Polyplacophora, Monoplacophra, Gastropoda, Bivalvia, Scaphoda, Cephalopoda.

Class-Aplacophora

Aplacophora are worm like animals, without shell, some are having spicules all over the skin. They are mostly found in deep water or in all ocean and exclusively benthic; rudimentary mantle cavity; crystalline style or nephridia.

Sub Class-Chaetodermomorpha (Caudofoveata)

The mantle covers the entire body and absent of foot occur. Bipectinate gills are located in the posterior of mantle cavity. Body shape is cylindrical. Body walls containschitinous cuticle and scale like calcareous spicules.About 70 known species are found. They consume microorganism as food. (e.g-Chaetoderma, Falcidens, Limifossor, psilodens, Scutopus)

Sub Class-Neomeniomorpha (Solenogasteres)

Worm like, shell less molluscs. It has a radula and it may bear more than one teeth per row so there is absence of central radula tooth. Elaborated salivary gland. They have a unique sense organ, vestibulum. True ctenidia is absent. During developmental many solenogasters are covered by a spiny scleritome comprising spines or scale like plates.

They consume bodily fluids or tissue of cnidaria and ctenophores. They do not use their radulae to rasp pray like other molluscs. About 250 species are described. (e.g-Neomenia, Proneomenia, Pruvotina, Rhoplacomenia, Epimensa, Dondersia, Chevroderma).

Class-Monoplacophora

This name explains that "bearing one plate". These are found at the bottom of the deep sea. With a single, cap like shell, body bilaterally symmetrical, dome shaped mantle, spirally coiled protochonch, foot broad and flat, with 8 pairs of pedal refractor muscles, gills are five pairs, nephridia six pairs, in a radder sac radula is present, intestine much coiled, two pairs auricle and a single ventricle is present in heart. Internal segmentation occurs. Monoplacophorans were known only from lower paleozoic fossils. Their unusual anatomies share a much evolutionary speculation. Their structures are limpet like. All over the world 15 described species in 6 genera: Vema, Moplacophorus, Neopilina, Rokopella, Laevipiina, Micropilina.

Class-Polyplacophora

Chiton: previously known as Amphineura. The Greek derived name Polyplacophora comes from the word Poly- many, placo- tablet, phoros- bearing. They are about 940 extant and 430 fossil species are recognized. Chitons are reference to the chiton's 8 shell plate. Chitons are fully marine which are contrast to the bivalves. They bear a protective dorsal shell which is divided into eight aragonite valves. The gridle are bearing scales and spicules. Between the body and the gridle mantle cavity is present. Heart is three chambered. The excretory system consists of a pair of nephridia. Mouth is located on the underside carry tongue like structure radula. Salivary glands are present inside the mouth cavity. For the capturing of pray cilia is present. Separated sexes; fertilization is external. They have a relatively good fossil record, which is 40 million back to the Devonian. They are about 6000 species described.

Order-Lepidopleurida

Primitive chiton belongs to this order. Usually posterior gill arrangement, simple gamet structure and asthete innervation (Sirenko 1993, 2006; Buckland- Nicks 2006; Sigwart 2008). Approximately, 130 living species are known within Lepidopleurida. It has shell plates and attachment with the teeth. Gridle are present over plates. It has few posterior pairs. (e.g-Lepidochiton, Lepidopleurus, Oldroydia, Choriplax)

Order-Ishnochitonida

Teeth attached with outer edges of plates. Gridle not extending partly over plates. Mantle groove occupied by ctenidia do not extend the full length of foot. (e.g-Acanthochitona, Crytochiton, Cryptoplax)

Class-Gastropoda

Gastropoda have the maximum number in molluscs species. There are 24000 terrestrial and 30000 marine described species are there. Till now 444 extinct species are there. They include mostly snail and slugs. They are also known as univalves. Some are live in freshwater and some are marine. Gastropoda distributed from Arctic and Antarctic zones to the trophics. Mostly gastropods covered by one piece of shell, which is coiled or spiraled. During development visceral mass and mantle rotate 90-180^0 on foot (torsion). Olfactory organs, eyes, stoocysts and mechanorecaptors acts as sensory organ. Nervous system includes peripheral nervous system and central nervous system. Radula helps to rasp the pray. Almost all marine molluscsbreath with the help of gill.

Mostly marine gastropods show external fertilization. the class is usually divided into 3 sub classes: Prosobranchs (marine snails), Opisthobranchs (marine slugs) and Pulmanates (terrestrial snails and slugs). After these arrangements also many revisionary schemes have been proposed.

Sub Class-Prosobranchia

Prosobranch means gills in front of the heart. They contain gills, mantle cavity and anus situated in front of their heart. They have separate sex. Their head generally covered by tentacles which bearing basal eyes; foot with creeping

planer sole and typically with corneous or calcareous operculum to close shell aperture upon retract of head and foot; radula variable or absent nervous system streptonurous.

Order-Archaeogastropoda

They are also known as Aspidobranchia. These are marine prosobranchgastropodamolluscs. They are mainly herbivores. Generally having two gills and a double chambered heart.Primitively with two hypobranchial glands, 2 osphradia, 2 atria and 2 metanephridia. 1-2 bipectinatectenidia, siphon is not present in mantle cavity. Sexes are separate. Male generally without penis. Nervous system weakly concentrated. Some are marine and some are fresh water species. This species is the poly phyletic grade. There are 26 families, including pleurotomaridae and scissurellidae (slit shelled molluscs, the most primitive living prosobranches: e.g- Perotrochns, Pleurotromaria, Scissurella); Haliotidae (abalones, Haliotis); Fissurellidae (keyhole limplets; e.g- Diodora, Fissurella, Lucopinrlla, Puncturella).

Order-Mesogastropoda

Mesogastropoda were prosobranchgastropoda mollusks. J.Thiele was first introduced this order in 1921 during his work. Shells are mainly porcelaneous and nannocreous. Operculum usually presented corneous, rarely calcified. Head contain a pair of cephalic tentacles and also basal eyes. Mantle cavity is asymmetrical by structure; which having anterior left in current opening basically elaborated into an inhalant siphon. Radula generally taenioglossate, occasionally lost. Most mesogastropoda are gonochoristic, which are forms with cocentrated ganglia. There are 100 families including marine and fresh water.

Order-Neogastropoda

Absent of nacreous layer; 1-3 teeth in each row with radula; 1 osphradium; radula rachiglossate or taxoglossate; mantle forms siphon, carried within siphonal canal; sexes are separate, male with penis; concentrated nervous system; chitinous, heart with left atrium only; right nephridium lost. About two dozen families of marine snails, including Buccinidae(whelks:e.g; Buccinum)

Sub Class-Opistobranchia

Sea slug; Detorted body; Shell reduced and thin, external and internal, or lost altogether; ctenidia and mantle cavity usually reduced or lost; usually without operculum; head with 1-2 pairs of rhinophores or tentacles; hermaphroditic; euthyneurous with various degrees of nervous system concentration. Primary marine benthic; some are fresh water species. Traditional (conservative) classifications include nine orders (and over 100 families) of opisthobranchs.

Sub Class-Pulmonata

Land snails and slugs. Mantle cavity forms lung with contractile opening; without ctenidia (except perhaps in Siphonaria); body detorted to various degrees; highly concentrated nervous system (euthyneurous); hermaphroditic; without larvae; mainly terrestrial and freshwater forms, a few marine species.

Order-Archaeopulmonata

Primitive pulmonates with spirally coiled shell, but no operculum;mainly littoral.

Order-Basommatophora

Shell variable, minuteor moderate-sized, generally spirally coiled (planospiral) or patelliform; usually without an operculum; eyes at bases of sensory stalks; freshwater and intertidal; includes freshwater limpets.

Order-Stylommatophora

Shell absent or present; if present usually spirally coiled and often partly or completely enveloped by dorsal mantle; eyes on tips of sensory stalks; terrestrial.

Order-Systellommatophora
Sluglike, withoutinternal or external shell; dorsal mantle integument forms a keeled or rounded notum; head usually with 2 pairs tentacles, upper ones forming contractile stalks bearing eyes.

Class-Bivalvia (Pelecypoda/Lamellibranchiata)
Clams, oysters, mussels, etc. Laterally compressed; shell typically of two valves hinged together dorsally by elastic ligament and shell-teeth; shells closed by adductor muscles; head rudimentary, without eyes or radula, but eyes and statocysts may occur elsewhere on body; foot typically laterally compressed, usually without a sole; 1 pair large bipectinatectenidia, used in combination with labial palps in ciliary feeding; large mantle cavity; posterior edges of mantle often fused to form inhalant and exhalant siphons; 1 pair nephridia. Basically Bivalvia are marine or freshwater molluscs and microphagous or suspension feeders. The class includes about 10,000 living species represented at all depths and in all marine environments.

Sub Class-Protobranchia
Ctenidia are 2 pairs of simple,unfolded, bipectinate, platelike leaflets suspended in themantle cavity. Primitive bivalves.

Order-Nuculida (Palaeotaxodonta)
Shell aragonitic, interior nacreous or porcelaneous; periostracum smooth; shell valves equal and taxodont (i.e., the valves have a row of short teeth along hinge margin); adductor muscles equal in size; with large palp proboscides used for food collection; ctenidia small, strictly for gas exchange; foot longitudinally grooved and with a plantar sole, adults without byssal threads; nervous system primitive, often with incomplete union of cerebral and pleural ganglia; marine, mainly infaunaldetritivores. (e.g., Malletia, Nucula, Yoldia)

OrderSolemyida (Cryptodonta)
Shell valves thin, elongate, and equal in size; uncalcified along outer edges, without hinge teeth; anterior adductor muscle larger than posterior one; ctenidia large, used both for gas exchange and feeding (e.g., Solemya).

Sub Class-Lamellibranchia
Paired ctenidia, with very long filaments that fold back on themselves so that each row of filaments forms two lamellae; adjacent filaments usually attached to one another by ciliary tufts (filibranch condition), or by tissue bridges (eulamellibranch condition).

Super Order-Filibranchia (Pteriomorphia)
Ctenidia with outer fold not connected dorsally to visceral mass, with free filaments or with adjacent filaments attached by ciliary tufts; shell aragonitic or calcitic, sometimes nacreous; mantle margin unfused, with weakly siphons; foot well developed or extremely reduced; usually attached by byssal threads or cemented to substratum (or secondarily free). Primitive lamellibranchs, including mussels (Mytilidae: e.g., Adula, Brachidontes, Lithophaga, Modiolus, Mytilus) and other clams, such as the ark shells (Arcidae: e.g., Anadara, Arca, Barbatia), glycymerids.

Super Order-Eulamellibranchia (Heterodonta)
Ctenidia with outer fold completely connected dorsally to roof of mantle cavity, with adjacent filaments attached by tissue bridges; shell generally aragonitic, without nacreous layer; shell valves equal to subequal, with a few large cardinal teeth separated from the elongated lateral teeth by a toothless space; mantle more or less fused posteroventrally and forming incurrent and excurrent apertures that are frequently drawn out onto siphons; foot usually lacks byssal threads in adult. Advanced bivalves, mainly marine, including three main groups (treated here as orders).

Order-Paleoheterodonta

Shell aragonitic, pearly internally; periostracum usually well developed; valves usually equal, with few hinge teeth; elongate lateral teeth (when present) are not separated from the large cardinal teeth; usually dimyarian; mantle opens broadly ventrally. About 1,200 species of marine and freshwater clams. Includes the nearly extinct family Trigoniidae (with fewer than six living species, in the Australasian region), and the family Unionoidea (freshwater bivalves: e.g., Anodonta).

Order-Veneroida

Usually thick-valved, equivalved, and isomyarian. Includes the following families: cockles (Cardiidae: e.g., Clinocardium, Laevicardium, Trachycardium), little heart shells (Carditidae: e.g., Cardita), giant clams (Tridacnidae: e.g., Tridacna), surf clams (Mactridae: e.g., Mactra), solens (Solenidae: e.g., Ensis, Solen), tellinids (Tellinidae: e.g., Florimetis, Macoma, Tellina), semelids (Semelidae: e.g., Leptomya, Semele), wedge shells (Donacidae: e.g., Donax), venus clams (Veneridae: e.g., Chione, Dosinia, Pitar, Protothaca, Tivela), and the freshwater families Sphaeriidae (e.g., Sphaerium) and Corbiculidae (e.g., Corbicula).

Order-Myoida

Thin-shelled burrowing forms with well develope siphons; shell with 0–1 cardinal teeth. Includes the soft-shell clams, shipworms, and others: families Pholadidae (piddocks: e.g., Barnea, Chaceia, Martesia, Pholas), Teredinidae (shipworms: e.g., Bankia, Teredo), Corbulidae (e.g., Corbula, Mya).

Sub Class-Anomalodesmata

Shells equivalved, aragonitic, of 2–3 layers, innermost consisting of sheet nacre; periostracum often incorporates granulations; with 0–1 hinge teeth, generally isomyarian, rarely amyarian; posterior siphons usually well developed; mantle usually fused ventrally, with anteroventral pedal gape, and posteriorly with ventral incurrent and dorsal excurrent apertures or siphons; ctenidiaeulamellibranchiate or septibranchiate (modified as a horizontal septum). Marine bivalves (including the septibranchs); having one order (Pholadomyoida) and basically 12 families, including the aberrant clavagellidae (e.g. Brechites), Cuspidariidae (e.g., Cuspidaria), Poromyidae (e.g., Poromya), and Pandoridae (e.g., Pandora).

Class-Scaphopoda

Tusk shells Shell of one piece, tubular, usually tapering, open at both ends; head rudimentary, projecting from larger aperture; mantle cavity large, extending along entire ventral surface; without ctenidia or eyes; with radula, proboscis, crystalline style; with paired clusters of clubbed contractile tentacles (captacula) that serve to capture and manipulate prey; heart absent; foot somewhat cylindrical. Nearly 400 living species of marine, benthic molluscs in eight families, including Dentaliidae (e.g., Dentalium, Fustiaria), Laevidentaliidae (e.g., Laevidentalium), Pulsellidae (e.g., Pulsellum, Annulipulsellum), and Gadilidae (e.g., Cadulus, Gadila).

Class-Cephalopoda (Siphonopoda)

Nautilus, squids, cuttlefish, and octopuses With linearly chambered shell, usually reduced or lost; if external shell present (nautilus), animal inhabits last (youngest) chamber, with a filament of living tissue (the siphuncle) extending through older chambers; body cavity large; circulatory system largely closed; head with large, complex eyes and circle of prehensile arms or tentacles around mouth; with radula and beak; 1–2 pairs ctenidia, and 1–2 pairs complex nephridia; mantle forms a large cavity containing ctenidia; which contain muscular funnel or shiphon through which water is forced, providing jet propulsion; tentacles of male modified for copulation during reproduction time; benthic or pelagic, marine; about 700 living species available in whole world.

Sub Class-Nautiloidea (Tetrabranchiata)

The pearly nautilus. Shell is external and bearing many-chamber,exterior porcelaneous, interior nacreous (pearly); 80–90 suckerless tentacles present in head ; 13-element radula; beak of chitin and calcium carbonate; funnel of 2 separate folds; 2 pairs ctenidia ("tetrabranchiate"); 2 pairs nephridia; eyes like a pinhole camera, without cornea or lens; nervous system rather diffuse; with a simple, primitive statocyst; without chromatophores or ink sac. Fossil record rich, but represented today by a single genus, the chambered or pearly nautilus (Nautilus), with five or six Indo-Pacific species.

Sub Class-Coleoidea (Dibranchiata)

Octopuses, squids, and their kin. Shell reduced, internal or absent; head and foot united into a common anterior structure bearing 8 or 10 prehensile suckered appendages (arms and tentacles), 1 pair modified in male for copulation; 7-element radula; with chitinous beak; funnel a single closed tube; 1 pair ctenidia ("dibranchiate"); 1 pair nephridia; eyes complex, with cornea and lens; nervous system well developed and concentrated; with a complex statocyst; with chromatophores and ink sac.

Order-Sepioida

Cuttlefish. Body short, dorsoventrally flattened, with lateral fins; shell absent or internal, calcareous, often chambered, straight, or coiled; 8 short arms, and 2 long tentacles with suckers borne only on spooned tips, and retractable into pits; suckers lack hooks. (e.g., Rossia, Sepia, Spirula)

Order-Teuthoida (Decapoda)

Squids have elongated body, tubular, with lateral fins; shell internal, reduced to cartilage-like pen; with 8 arms and 2 elongate nonretractable tentacles; suckers often with hooks. Numerous families and genera. (e.g., Architeuthis, Bathyteuthis, Chiroteuthis, Doryteuthis, Dosidiscus, Gonatus, Histioteuthis, Illex, Loligo, Lycoteuthis, Octopoteuthis, Ommastrephes)

Order-Octopoda

Octopuses basicallyhaving short and rounded body, usually absent of fins; internal shell is vestigial or absent; 8 similar arms joined by web of skin (interbrachial web); most are benthic. About 200 species are found in whole world. (e.g., Argonauta, Octopus, Opisthoteuthis, Stauroteuthis)

Order-Vampyromorpha

The vampire squid. Body is plump like, with 1 pair of fins; shell reduced to thin, leafshaped, uncalcified, transparent vestige; 4 pairs equalsized arms, each with one row of unstalked distal suckers; arms connected by extensive web of skin which is bearing interbrachial membrane; fifth pair of arms represented by 2 tendrillike, retractable filaments; hectocotylus lacking; radula well developed; ink sac degenerate; mostly deep water.(one living species, Vampyroteuthisinfernalis)

Values of Molluscan Diversity

The relationship between molluscs and man has been very old since prehistoric time. Discarded shells were found in the kitchen middens and in the excavations of stone age culture. There are evidences that shell trade existed in protohistoric Iran and southern Asia (Durante, 1979). For the primitive man shells were strange and rare objects. Due to beauty of shells, the primitive man collects them up from sea beach and the wondering tribes carried them inland. The inland people were never imagin such objects so they accept it with curiosity. As the associating grew man attributed magical and mythical powers to shells and had also started manufacturing various articles out of them.

Aesthetic value

Due to colourful exterior and for the perfect shape which is mostly consist of spiral curve a shell appeal to human eye. Gastopoda, Bivalvia, and Nautilus in cephalopoda attracted men from the initial period.

SubbaRao: Indian sea shell: Polyplacophora and Gastropoda

Shell of snails is not mathematical perfection but also beautiful and regular, efficient. One of the best examples of formation of spiral curve is the growth shells in snail. That means in this growth the size will increase but the geometric proportions will not occur. In molluscs there are two types of important spiral or spiral of Archimedes and the equiangular spiral or logarithmic spiral. French philosopher Descartes in 1638 named it equiangular spiral and Jacques Benoulli in 1691 named it logarithmic spiral. Its fundamental property is to govern the growth of shell of the molluscan.

Geometrical Symmetry-Nautilus

Nautilus basically found in Andaman Nicobar and they are aesthetically appealing and geometrically perfect. There are 38 chambers in adult Nautilus in which first four are formed within the egg and further chambers are develop in every 2 to 3 weeks. These are based logarithmic or equiangular spiral. Length of shell during growth increase with proportionate of radius so that it can be unchanged.

Cones

Cones are not only known for its beautiful colour and shape but for aristocrats. Collection of cones considered as pride possessions. There are about 400 species of cones. Two rare cones are also known as 'Glory of the sea'. These are *Conusgloriamaris;* Chemnitz (1777) and *Conusmilneedwardsi;*Jousseaume(1889) known as glory of India. There are other 27 species of cones which are important because of there poisonous nature. There poison is equivalent to the poison of cobra. In India 5 species are found they are *Conusgeographus*(Geography cone), *C.aulicus*(princely cone), *C.marmoreus* (marble cone),*C.tulipa*(tulip cone) and*C.textile*(textile cone) found in the reefs of Andaman and Nicobar islands, in Lackshadweep. From these five species *Conusgeographus* is one of the dangerous species.

Cowris

Cowries are associated with man aesthetically or ornamentally and financially. In primitive time women were use it as their ornaments. That time they also belief that cowry has the power of conferring fertility and it became the symbol of womenhood. Cowries are also used as the charms against the evileye and also in that time villagers also tie these to the horse and bulls.

Commercial Value

There are two types collection of shell, these are commercial shells and collector's shell or specimen shells. Commercial shells and collector shells are basically used in shell craft industry after polished and cut into various sizes. India have risen sea shell exports 20 tons in 1969 to 466 tons in 1979 (Wells, 1981). The Philippines is the leading exporter of sea shells with around 80% followed by South Korea, Thailand, Taiwan and Mexico. India has a 5% in a few years. Basically shells are collected from Tamil Nadu coast, Kerela, Andaman and Nicobar Islands and collection from Odisha, it was became late. It was reported that one shell craft Industry in Bombay processes around 1200 tons of seashells annually of this about 200 tons are thrown away since the shells do not conform to certain standards of colour, shape and size.

Raw Material for Shell Crafts

Sea shells are used in making house hold stuffs table lamps, ashtrays, agarbati stands, door hangings etc. These are also used in lime industry, poultry feed additives. Due to the large size and glittering surface when polished turban shells and top shells are popular.Chank was used as ornaments during Mahenjodaro and Harappa time. Pearl is nothing but a biochemical product of molluscs. Pearl is used as mostly in crafts and ornamental field.

Biomedical Value

From era of Ayurveda, molluscs are used in preparing medicines. Extracts, powder of oyster shell, cowry shell also use in homeopathic medicines. For the skin disease to rickets and asthma sankhabhasma is used. Molluscs also provide biologically active compound in marine diversity. For the biomedical potential molluscs, molluscs secrete secretions from the dermal region or form internal glands.

Marine Biodeterioration

A number of marine bivalves attached with hard substances inside the ocean. Where attached bivalves made considerable damage. The magnitude of the problem of biodeterioration is such that in spite of several years of research. Bivalvia Molluscs are the most successful as followers and borers.

Evolutionary Character

Molluscs are among the best-known animals on the planet earth as they have conquered almost all terrestrial and aquatic habitats of the earth. The dramatic variations over their body plan morphology make them an ideal group for comparative studies into how evolution has brought about phenotypic diversityfrom a common ancestor that roamed the oceans' floors at least 550 million years ago (Haszprunar G &Wanninger A, 2012.) Molluscsevolutionay history with the occurance of mineralized exoskeletal hard parts in their body plan has given a rich fossil record, at least of the shell bearing taxa (Parkhaev;2008,2017). Some findings together with molecular clock estimates revealed a picture according to which all major molluscan sublineages are deeply rooted in the Cambrian (Vinther;2014,2015).

Shell Parts

The calcareous hard shell of mollusc is meant to support and protect the soft body of the organism. Ancestral Mollusc is thought to have had a shell but gradually its been reduced or lost in some family members of mollusc such as octopus, squid, solenogasters and caudodoveat etc. The scientific study of molluscs is commonly known as malacology while conchology is a branch of it that deals specially with the study of shells. Every shell bearing mollusc is not bound to be marine; it can be in terrestrial or freshwater regions. There is also a wide range of variation in the shape, colour, pattern and ornamentation of shell even within some species of mollusc.

Nearly all five main classes of molluscs have a shelly covering. Most of the seashells belong to two main classes, Gastropoda (about 80%) and Bivalvia. The gastropods have a single piece of shell, which is usually coiled at axis. Bivalves have two pieces of shell hinged together. Bivalves have two pieces of shell hinged together. Other shells are tusk shells that are relatively similar (Class- Scaphopoda), a few Cephalopoda (family- Nautilidae) have shell and the chitons has 8 articulated pieces or valves (Class-Polyplacophora).

The Bivalve shells have left and right valve connected by a ligament, which is visible, when valves are closed. Shell shape, sculpture, cardinal complex, hinge teeth, shape of pallial line, pallial scars and adductor scar are considered as important characters for the identification of bivalves.

Objectives

There are few mentionable studies or literatures available on molluscan diversity around the coasts of Puri district, specifically in sea shore. Therefore, my study on the selected coastal connecting area of Puri district (Baliharchandi) will provide some better knowledge of the presence of rich molluscan fauna.

MATERIALS AND METHODS

Search method was adopted, it was conducted for two months from November to end of December 2019 by selecting the mouth area, upper reaches and connecting channels of Baliharchandi estuary and from Puri sea beach to complete the study.

Study Site

The study was conducted in the connecting channels of Baliharchandi estuary (fig.4). Baliharchandi beach is 27 km to Puri. It famous for its clean beach and Baliharchandi temple (fig.5). It is located at eastern coast of Odisha(fig.3). The site is the connected area of the river Bhargavi and Bay of Bengal sea. Connected areas are intertidal mudflat area. Coastal areas are filled with Eucalyptus and Jhaun plants which keep the site moist and suitable home for molluscs (fig.6).

Collection

There are many ways to collect molluscs or shells. It can be collected from other collectors or from the sea dealers or fisher man by purchase it. My collection is done directly from natural habitat. During low tide period, they are buried inside the mud in the presence of sunlight. So my collection of sample were made during low tide period. live specimens or dead shells were collected by hand picking method. and digging the substratum where the surface was intertidal mud flat. Then they were washed in the salty water at the collection site to remove impurities and mud. The number of samples varies from 1 to 65 depending upon their abundance. Polythene bag was used during collection period at the study sites. A certain code of ethics followed during the collection.

Code of ethics for collection

- Collection was done in the areas where collections are permitted without making any disturbance to their habitats.
- Minimum number of species were collected without making any indiscriminate collection and putting devasting effect on the local population.
- Local, national, and international laws governing species are habitats were not included.
- Species in their reproductive stage and juvenile stage are not collected at all.

Identification

The identification of the collected species based on their morphological character, shell pattern, shape, and size. Taxonomic monographs of Vaught (1989), Bouchet and Racroi (for gastropodas), Bieleretal. (for bivalve and polyplacophora).

Preservation

After studying the morphological character, live specimens were fixed with 5% Formaline solution and brought to the laboratory (fig-9). They are finally preserved in Glycerine ethyl alcohol mixture in the ratio of 1:19 as recommended by Gosner (1971). Dead shells are washed, dried and kept in plastic box or card board box. Each specimen were photographed before their preservation with the help of good quality phone (VIVO-Y69).

RESULTS

Teleoscopiumteleoscopium; Linnaeus, 1758.
Class- Gastropoda
Order- Caenogastropoda
Family- Patamidiae
Genus- *Teleoscopium*
Sample collected- 28 no.
Measurement–130 mm
Diagnostic Character : Shell very large, up to 130mm in length, elongate, with about 14 flat sided whorls. Aperture with thickened lips, outer lip arched and curved over short siphon canal, columella with callus deposit, posteriorly thickened with rib like callus.

Outer lip also with callus, interior or aperture absolutely grooved. Sculptured with deeply incised regularly spaced spiral grooved separated by broad and flat inter spaces, straight edged and flattened transpiralribsin juveniles, a humped varix on the body whorl anteriorly opposite columella. Colour dark brown, interior purple brown (SubbaRao NV 2003).
Place of collection – Baliharchandi, Puri

***Nerita balteata*(Sea snail);** Muller, 1774.
Class- Gastropoda
Order- Neritimorpha
Family-Neritidae
Genus- *Nerita*
Sample collected- 2 no.
Measurement – 11.5-33.8 mm
Diagnostic Character- The length of shell is 11.5- 33.8 mm. Shell is medium large in size, sculptured with deeply regular spaced spiral grooves, upper surface is bulging, colour brown to vary purple.
Place of collection- Baliharchandi, Puri

Notocochlis tigrine; Roding, 1798.
Class- Gastopoda
Order- Littorinimorpha
Family- Naticidae
Genus- Notocochlis
Sample collected- 4
Measurement length- 35mm
Diagnostic Character- length is of 35 mm. Shell triangularly ovate and think, umbone is pointed and curved; sculpture with concentric striae, strong at the ventral margin. Ligament small, lunule large, superficial, almost absolete. While in colour or with some tinge of rust brown (Dey and Anirudha 2008).
Place of collection- Baliharchandi, Puri

Cerethidea cingulata;Gmelin, 1791.
Class- Gastropoda
Order- Caenogstropoda
Family- Potamididae
Genus- *Pirenella*
Species collected-60
Measurement length- 7.85 to 20mm
Diagnostic Character- Length is form 7.85 to 20mm. Shell is tiny. Body whorl anteriorly opposite collumela, dark and light brown in inner surface smooth, glossy outer surface with lines and radial striae; adductor central; umbo small, inconspicuous, cardial teeth two, ridge like, diverging from the umbo at a narrow angle; unequal and the posterior larger. (SubbaRao NV 2003)
Place of collection- Baliharchandi, Puri

Neverita didyma; Roding, 1798.
Class- Gastropoda
Order- Littorinimorpha
Family- Taticidae
Genus- *Neverita*
Sample collected- 1
Measurement length- 57 mm

Diagnostic character- The length is 57 mm, size of shell is large, body whorl large and inflated. Outer surface is smooth and glossy. Aperture large and semiovate, Columella with a large transversely expanded curved callosity divided into two by a transverse groove, posterior portion large and fuses with the body whole covering the umbilicus, anterior part smaller and free. Surface uniformly pale brownish or grayish, callosity and anterior of aperture deep chestnut (SubbaRao NV 2003).
Place of collection- Baliharchandi, Puri

***Coenobita*(Hermit crab);**Latreille, 1802.
Class- Malacostraca
Order- Decapoda
Family- Peguroidea
Genus- Coenobita
Sample collected- 1
Measurement length – 29 to 80 mm
Diagnostic character- Larger shell; spirally curved and calcified abdomen; tip of abdomen clasp strongly on to the columella. Antenna is larger outer pair compound eyes are comprised of faceted lenses. Orange or red legs, bluish grey in colour.
Place of collection- Baliharchandi; Puri

Archachatina marginata; Swainson, 1821.
Class- Gastopoda
Order- Heterobranchia
Family- Achatinidae
Genus- Archachatina
Sample collected- 1
Measurement length – 210 to 130 mm
Diagnostic character- The snail has a bulbous, large, and broad protoconch with a white orbluish white columella, parietal wall and outer lip. The shell has the appearance of a woven texture.
Place of collection- Baliharchandi, Puri

Viviparus contectus; J.E Gray, 1847.
Class- Gastopoda
Order- Caenogastropoda
Family- Viviparide
Genus- *Viviparus*
Sample collected- 1
Measurement length – 25to35mm
Diagnostic character- The shape is bulbous, large and broad protoconch, brown columella, parietal wall, and other lip. The colour is dark greenish brown or greyish yellow with three reddish brown spiral bands and striated. Shell apex is burnt and weakly having convex whorls. The last whorl is relatively larger. The umbilicus is narrow. The operculum is attached to the dorsum and the rear foot. Body is wide and T shaped and mouth has radula. There a pair of present short tentacles; the eyes are on the external side of each tentacle.Place of collection- Baliharchandi, Puri

Ellobiidae; MelampidaeStimpson, 1805.
Class- Gastopoda
Order- Heterobranchia
Family- Ellobidea
Genus- *Ellobiidae*

Sample collected- 1
Measurement length- 15mm
Diagnostic character- Known as hallow- shelled snails, terrestrial pulmonate gastropod mollusks. Covered with hard shell, spirally curved body, bulbous, large and broad protoconch, brown and black in colour.
Place of collection- Baliharchandi, Puri

Littorina obtusata; Linneaeus, 1758.
Class- Gastropoda
Order- Caenogastropoda
Family- Littorinoidea
Genus- *Littorina*
Sample collected- 1
Measurement length- 13.5mm
Diagnostic character- Shell is 13.5mm in length, commonly known as flat periwinkle. The snail is medium large, bulbous cover, compact shell covers the mantle cavity, the shell colour is brown.
Place of collection- Baliharchandi, Puri

CONCLUSION

During the present study, a total number of 133 examples of specimens are collected. After the study, it is found that these samples are belong to 17species. There are two major classes in my study Gastropoda and Biavalvia. From the 17 species, 13 species belongs to Gastropoda and 4 species belongs to Bivalvia. In my study the no of *Cinguata*which is more than other species that is 60 in number.

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REFERENCES

1. Anonymous (2011) Clasiification of Mollusca. www.biologyeducation.net.
2. Chandra A and Chakraborty SK (2008) Distribution, density and community ecology of macrobenthic intertidal polychaetes in the coastal tract of Midnapore, West Bengal, India. Marine Biological Association of India, 50(1): 7-16.
3. Chapman AD (2009) Numbers of Living Species in Australia and the World. Australian Biological Resources Study, Canberra ,2ndedition,pp 200-260.
4. Datta SN, Chakraborty S K, Jaiswar AK and Venkateshvaran K (2008) Temporal and spatial differences in species diversity in the intertidal region of south Mumbai. Marine Biological Association of India, 50(1): 29-37.
5. Dey A and Ramakrishna (2007) Fauna of Andhra Pradesh, State Fauna Series. Record of zoological Survey of India, 5(Part-7)-Marine Molluscs, pp 149-260.
6. Dey and Anirudha (2008) Commercial and Medicinal Important Molluscs of Sundarbans, India. Record of zoological Survey of India, 286: pp 1-54.
7. Dey M, Jamadar A and Mitra A (2005) Distribution of intertidal malacofauna at Sagar Island. Records of the Zoological Survey of India, 105(2): 25-35.
8. Haszprunar G and Wanninger A (2012) Molluscs. Current biology 22 :510-514.

9. Hayward PJ, Wigham GD and Yonow N (1990) Mollusca Polyplacophora, Scaphopoda, and Gastropoda. The Marine Fauna of the British Isles and North-West Europe. ed. PJ Hayward and JS Ryland. 628-730.http://www.marinespecies.org/
10. Kumar PS and Khan AB (2013) The distribution and diversity of benthic macroinvertebrate fauna in Pondicherry mangroves, India. Aquatic biosystems,9(1):15.
11. Manoharan J, Varadharajan D, Thilagavathi and Priyadharsini S (2011) Biodiversity and abundance of benthos along the South East coast of India.Advances in Applied Science Research, 2(6): 554-562.
12. Mantosh Das and JoydevMaity (2018) Availability and utilization of molluscs at Dighacoast,East coast of India. International journal of biology Research. 3: 3, pp 46-53.
13. Mitra A, Choudhury A and Bhattacharya DP (2001) Preliminary observations on macrobenthcmolluscan diversity in relation to physico-chemical variables in Bay of Bengal coast. Journal of Indian Fisheries Society of India, 33(2): 73-76.
14. Mitra S, Sarkar J (2002) Report of living pen shell Pinna (Atrina) pectinatapectinatalinnaeus (mollusca: bivalvia: pinnidae) from shankarpur, west Bengal, Records of the Zoological Survey of India. 100 (Part 3-4): 229-23.
15. Morton JE (1958) Molluscs. London: Hutchinson University Library, pp-11.
16. Parkhaev PY (2008) The early Cambrian radiation of Mollusca. In Phylogeny and Evolution of the Mollusca eds W.F Ponde and D.R Lindberg, pp 33-70.
17. Parkhaev PY (2017) Origin and the early evolution of the phylum Mollusca. Paleontological journal, 51: 663-686.
18. Ramakrishna and Dey A (2003) Manual on the Identification of Schedule Molluscs From India,Zoological Survey of India, pp 1-40.
19. Richard C Brusca and Gary J Brusca (2002) Invertebrates. Sinauer Associates, Inc., 2nd ed, pp 702-715.
20. SubbaRao NV (2003) Indian Seashells (Part-I): Polyplacophora and Gastropoda. Record of zoological Survey of India. 192: i-x, pp 1-416.
21. SubbaRao NV, Dey A and Barna S (1992) Estuarine and Marine Mollucs. State Fauna Series 3. Fauna of West Bengal. Zoological Survey of India .9: 129-268.
22. SubbaRao NV, Dey A and Barua S (1995) Mollusks in Hugli-Matla Estuarine Ecosystem Series Zoolgical Survey of India. 2:41-90.
23. Surya Rao KV and Mitra S (1998) Mollusca, Fauna of Mahanadi Estuary. Estuarine ecosystem series 3, Zoological Survey of India, 161-197.
24. Tudu PC, Yennawar p, Ghorai N, Tripathy B, Mohapatra A (2018) Indian Journal of Geo Marine Science, 47(08), pp 1537-1560.
25. Varadharajan D, Soundarapandian P, Gunalan B and Babu R (2010) Seasonal abundance of macro benthic composition and diversity along the South East coast of India. European Journal of Applied Sciences, 2(1): 1-5.
26. Vinther J (2014) A molecular palaeobiological perspective on aculiferan evolution. Journal of Natural History 48: 2805-2823.
27. Vinther J (2015) The origins of molluscs. Palaeontology 58:19-34.
28. Winck worth R (1940) New species of shells from Madras. Procmalacsoc London. 24:19-49.

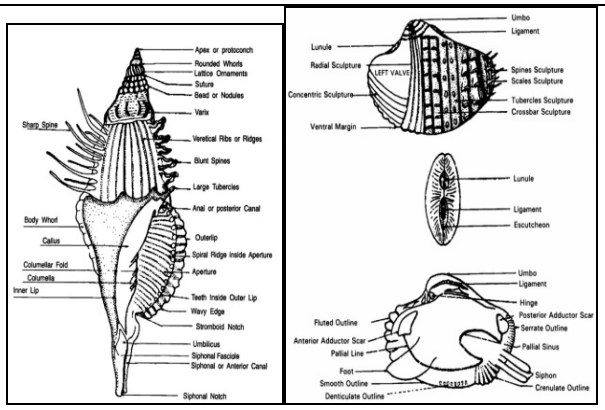

Figure 1. Hypothetical Gastropod, Bivalve shell showing the most common features.

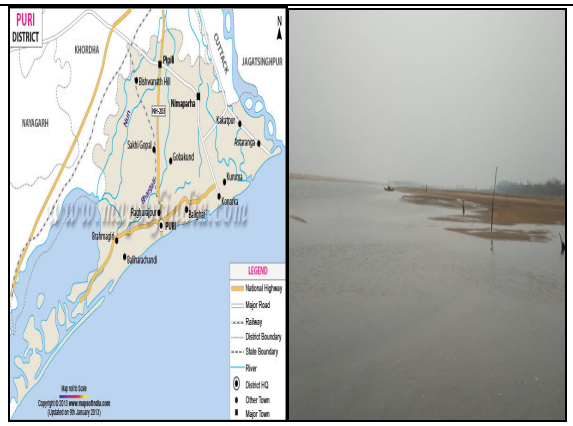

Figure 2. Location of Baliharchandi, Puri

Figure 3. Collection of *Telescopium telescopium* and *Pirenella cingulate*.

Figure 4. Dorsal and ventral view of *Teleoscopium teleoscopium*.

Figure 5. Dorsal and ventral view of *Nerita balteata*.

Figure 6. Dorsal and ventral view of *Notocochlis tigrine*

Figure 7. Dorsal and ventral view of *Cerethidea cingulate*.

Figure 8. Dorsal and ventral view of *Neverita didyma*.

Figure 9. Dorsal and ventral view of *Coenobita* (Hermit crab).

Figure 10. Dorsal and ventral view of *Archachatina marginata*.

Figure 11. Dorsal and ventral view of *Viviparus contectus*.

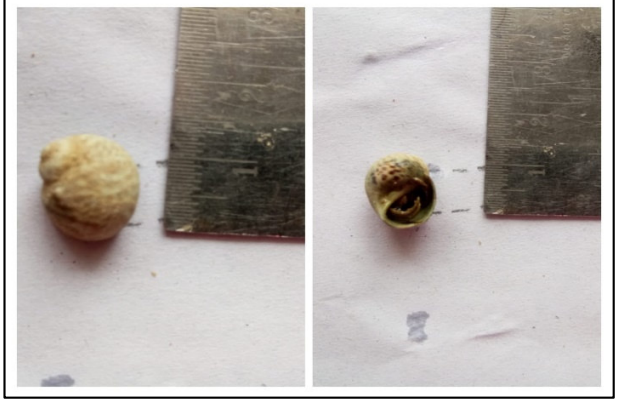

Figure 12. Dorsal and ventral view of *Ellobiidae*.

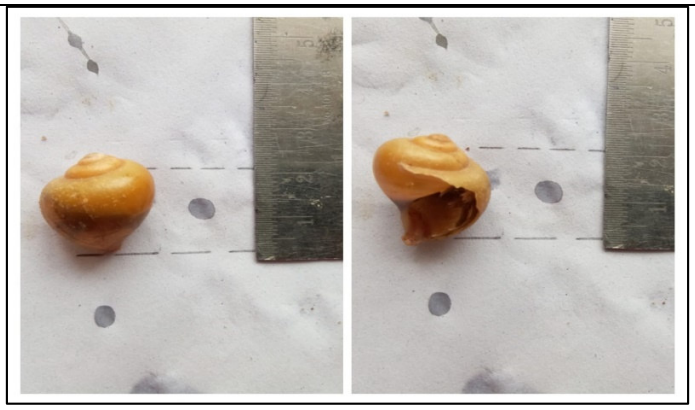

Figure 13. Dorsal and ventral view of *Littorina obtusata*.

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RESEARCH ARTICLE

Real-time Object Detection and Recognition Using Deep Learning with YOLO Algorithm for Visually Impaired People

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ABSTRACT

This paper aims at combining real-time object detection and recognition with suitable deep learning methods in order to detect and recognize objects position as well as the names of multiple objects detected by the camera using an object detector algorithm. This is to aid the visually impaired user without the help of any other person. The image and video processing algorithms were designed to take real-time inputs from the camera, Deep Neural Networks were used to predict the objects and uses Google's famous Text-To-Speech (gTTS) API module for the anticipated voice output precisely detecting and recognizing the category or class of objects and locations contained. Our best result shows that the system recognizes 91 categories of outdoor objects and produces the output in speech i.e. in an audio format even when a reduced amount of spectral information from the data is available.

Keywords: COCO dataset, Deep Neural Networks, gTTS, Object detection, object recognition, YOLO algorithm

INTRODUCTION

A human being's best basic feature is often his ability of vision. The ability of being able to see things with our eyes is regarded as a gift and is the primary factor in our day-to-day activities [1]. A major challenge in many of the visually impaired people is they are unable to be completely independent and are limited by their vision. The visually impaired people face trouble with such activities and object recognition will be an imperative feature they can depend on a regular basis. They usually face challenges in the identification of items and movement in the

surroundings especially while walking on the streets. According to a World Health Organization (WHO) in October 2019, "Globally, at least 2.2 billion people have a vision impairment or blindness". The majority of people with vision impairment are over the age of 50 years [2].

Limited applications have been developed to assist the visually impaired people. However, the absence of actual real time object recognition with voice output for the visually impaired people is still not widely modernized. Some of these applications are centered on sensing obstacles near the user and alerting them through alarms or beeping sounds with the implementation of Internet of Things (IoT). For different purposes, a number of gadgets are required to hold by the users. For instance, smart sticks with obstacle detector, mobile phones, navigators, etc. are required for navigation assistance. These devices are expensive and could be a hindrance to the user at times. Some of the alternatives that are widely used today to provide assistance to visually impaired people are: Tactile signs and Braille texts that are labeled on the top of the items for the identification [3, 8]. High-tech systems such as Radio Frequency Identification Devices (RFID), barcodes or talking labels that can be used to find objects in near distance [4, 8].

Normally, complete visual impairment or low vision people face difficulties in outdoors. Voyaging or strolling down in a jam-packed road may represent an incredible trouble. In general, a visually impaired person takes support from their family members or sighted friends to maneuver through unfamiliar environments as well as to avoid the obstacles. For all these obstacles, they use canes. But, a cane cannot verify the kind of object ahead of them. From their experience, blind people usually identify an object, which leads to an injury or accident if an object is not quite the same as the one anticipated. They may also come across items such as stairs, dogs, parked cars, bicycles etc. that are hard to evade when walking along a walkway. The most challenging portion of such kinds of applications is the precise recognition of the objects and their positions appropriately. To recognize any object, those applications take an image as the input and convert that image into a grayscale formatted image. After formatting into grayscale photo, they run a top-down or bottom-up inspection and extract it into a histogram, which is based on pixel color depth.

A huge number of researches have been carried out in the realm of real time object recognition using Deep Learning. In various ways, the Automatic detection of objects in image as well as in video process has been executed. Few are similar to our proposal method. All these researches can be distinguished in the detection of objects in any environment. In total our proposed methodology will detect 91 categories of objects including the indoor, outdoor and electronic devices.

In the year 1985, the first research paper on a guidance system was written and published by Jack Loomis who was a Professor of Psychology at the University of California. It was based on a GPS tracking system and started the research on navigation system for visually impaired people [5]. In the year 2009, a South Korean team designed a prototype of Unmanned Underwater Vehicle (UUV). On that UUV, a camera and a laser beam were operated to detect any obstacle in its path. The camera captured the images and the laser marked on it. Then it was converted into grayscale images. Using the most enlightened pixel and histogram, it could detect any object in front of the Unmanned Underwater Vehicle [6]. This popularized the method of obstacle detection. In the year 2018, R. Gnana Bharathy presented a context of object detection and classification using video analytics in cloud that precisely resulted in a high performance. Here, a cascade classifier is used to automate the video stream analysis process and laid the basis for the experiment of a large kind of video analytics algorithms [7].

In paper [8], presented the chief characteristics of software modules dedicated to help the visually impaired or blind users. The main objective is to less use of separate devices for object recognition and motion detection. These modules are implemented for Android operating system, due to the major use of smart phones in day to day life. Object recognition and the motion detection module are two trainable (ANN based) modules. This paper described the Image processing algorithms to identify the objects and detect the motion of objects. In this system, notifications

are provided to the users in the form of verbal messages. In this paper, our main focus is to help the visually impaired people for recognizing the objects by implementing machine learning for a product. It will be very helpful for the visually impaired people to feel less visionless. The paper is organized as follows: In section II, we discuss our proposed method for object recognition module. In section III, we talk about the experimental result. Eventually, we reach with our conclusion and future scope in section IV and V.

Proposed Methodologies

Object Detection and Recognition

Object detection and object recognition are related methods for object identification; however, they differ in execution. While both are extensively used for image and video processing, object detection is said to be a subset of object recognition. Object detection and recognition are widely used in the vast range of industries from individual security to productivity in the work environment. It is applied in various fields of computer vision as well as automated vehicle systems, machine inspection, surveillance, security, and image retrieval [18]. Generally, the non-operating system devices can not recommend the text to speech conversion function. Thus, the most mainstream decision of smart phones with visually impaired users is either Android based phones or an iPhone.

Object detection: Object detection is the process of finding instances of objects in images and videos where the objects are located in the specified image or video. It highlights the recognized objects with bounding boxes and their position in the frame. Object detection is a technology which relates to image processing as well as to computer vision. It defines and detects various objects, for instance, animals, vehicles and persons from videos and digital images. Object detection has the ability to categorize several objects quickly within a video or digital image. Object detection has been around for decades, however is getting increasingly evident over a scope of industries now, like never before previously. Various methods have been used to implement the object detection system. However, this paper uses deep learning technique to provide high and better accuracy for object detection of varied object categories or classes [18]. The Object Detection Process is as shown in Fig. 1, which illustrates the detection of objects in step by step starting from process of Classification, Localization and object Detection.

Object recognition: Object recognition is a significant skill essential for most computer and robot vision classifications. It is an important visual perception task used in image and video processing using computer vision.

Deep Neural Networks (DNNs)

In this paper, Deep Neural Networks (DNNs) methodology is used to train our model to recognize the items according to their labels. DNNs are very powerful and important machine learning model. The basic working model of DNNs is as shown in Fig. 2.

With the help of DNN, we not only classify the items but also train it to estimate the precise location of the detected item. To achieve that, first we formulate a DNN-regression. In second, provide a multi-scale box inference and after that a refinement step to produce precise detections. DNN-regression gives a binary mask of the object bounding box. After that, extract detections from the masks by using a bounding box to as shown in Fig. 3. The next step is to increase the localization precision, which applies a DNN mask generation in a multi-scale fashion on a small number of large image crops as well as on full image, succeeded by a refinement step as shown in Fig. 4. Therefore, this paper can apply a DNN to predict a low-resolution mask, limited by the output layer size, to pixel-wise precision with small effort – the network shall apply on a few dozen times per input image [19]. The authors of [19] have presented a method which is quite simple for object detection using DNN-regression. The simplicity of the model provides a benefit of easy applicability to a varied of categories. Thus, in detection, DNN has an overall better performance.

Yolo Algorithm

Joseph Redmon first proposed the YOLO algorithm along with his team. He published his paper on YOLO in 2015 which was titled "You Only Look Once: Unified, Real-Time Object Detection" and immediately was a huge success. YOLO is a Convolutional Neural Network (CNN). The algorithm "looks once" at the picture in the context that making predictions involves just one forward propagation that passes through the neural network. YOLO model is faster efficiently than any other method of detection of objects. YOLO's greatest advantage is their speed. This takes 45 frames per second. The model is built in such a succinct way as to familiarize its network with abstract description of items [11]. The flowchart i.e. working procedure of YOLO algorithm for real time object recognition is illustrated in a flowchart as shown in Fig. 5. The recent studies on implementing object recognition into the real world has been proved to be quite beneficial and efficacious. For recognizing the instances of an object or images, which belongs to an object class, is done by object detection methodologies. These methodologies frequently apply extracted features and learning algorithms for recognition process.

The main target of object detection is to localize a particular or more objects from videos or digital images. On the contrary, Object class recognition acts on categorization of objects into a specific category or a class. All objects has its own characteristics, which helps to recognize the similar objects in other videos or images. Also makes them differentiate from other classes [18]. Object detection, detects and define objects, for instance, persons, animals, things, vehicles and so on. In order to achieve object recognition, we have to combine You Only Look Once (YOLO) architecture algorithm and Common Objects in Context (COCO) dataset that achieves a fast and efficient deep learning method.

Proposed Architecture

Our proposed system contains a camera, computer and headphones. The lens of the camera captures frame by frame through real time video processing, then the algorithm detects objects using Darknet module, the program identifies them from the given You Only Look Once (YOLO) trained dataset named COCO and the output is given by the speakers or headphones, whichever is convenient and is available to the user at that moment. Here, completely we apply a deep learning-based methodology to lessen the issue of vision using object detection with a speech output in an end-to-end fashion as shown in Fig. 6.

YOLO is designed for complete picture processing and improves the efficiency of object detection in an unswerving way. Here, the frame detection is taken as a regression problem. The networked is focused on fresh photographs and YOLO uses the whole background during training and testing periods such that it encodes specific knowledge regarding groups and their appearances subtly. It uses features from the whole picture to simultaneously predict all bounding boxes across all groups for an image. The method splits the input picture into a pattern of S x S. when the center of an item falls into a grid cell, the grid cell can detect the point and determine the confidence scores for those boxes. When there is no item in that cell, then the confidence scores will be 0. These bounding boxes are calculated according to the estimated probabilities [11]. Fast YOLO uses a neural network with less convolution layers, that is to say 9 out of 24 layers, and less filters in those layers. YOLO forecasts several bounding boxes per cell on the grid. After non-max suppression where each item is identified once, it then generates known items together with the bounding boxes. The algorithm outperforms other top detection algorithms [12].

In Paper [13], Redmon and Farhadi carried out further work, "YOLO900: Better, Faster, Stronger." They made a range of enhancements to the YOLO detection system including the identification of over 9000 types of items by jointly improving detection and classification. More recently, in paper [20], the same researchers published another paper on their development with YOLO advancing much further, "YOLOv3: An Incremental Improvement". This is the version we have used for our paper.

Speech Output using gTTS API

The speech output module, that uses the speakers or headphone or a Bluetooth ear piece, has been added specifically to alert or simply let the user know about the surrounding objects around or in front of them. In addition to that, Speech Output would be more beneficial and faster at navigation especially when the user is walking in the streets. Hence, visually impaired individuals will take required preventive steps or stop for a short while till the objects ahead of them move out. This module works by using Google's Text-To-Speech (gTTS) API, which is widely used in android smartphones. It is a screen reader program that Google has built for Android operating system. With the help of several languages such as German, French, Tamil, Hindi, English and many more, gTTS powers functions to read out loud the text on the screen. All these languages support in gTTS API. It was released on 6 November 2013. The speech is delivered in either fast audio speed or slow speed. Nevertheless, as of the most recent update, the voice of the created audio cannot be altered.

The python module gTTS that we use in our system basically creates an audio file from spoken text via the gTTS API. The length of the spoken text is unlimited by tokenizing long sentences where, naturally, the speech would pause. This API has the best advantage of sounding very natural [14].

RESULTS AND DISCUSSION

Dataset

The experimental result uses COCO dataset, which is a large-scale object detection, segmentation, and captioning dataset. The dataset of Microsoft Common Objects in Context (MS COCO) includes 91 common categories of objects, 82 of which have more than 5,000 named instances. In total, there are 2,500,000 instances labeled in 328,000 pictures. Unlike the common ImageNet dataset, COCO has less categories but more instances per category. This can help to learn complex object models capable of accurate 2D location. The dataset is also considerably bigger than the PASCAL VOC and SUN datasets according to the number of instances per category [15].

In [15] utilized a joint training on both the datasets i.e. ImageNet as well as COCO dataset to train YOLO9000. The outcome is a YOLO model, named as YOLO9000, which will predict the detected object categories without a labeled data [15]. The COCO dataset consists of 91 labels such as:

Kitchen and dining objects including spoons, knives, forks, cups, wine glasses, [16] etc.
Animals including sheep, cows, horses, birds, dogs, cats, etc.
Stop signs and fire hydrants
Cars and trucks
Airplanes
Bicycles
People

The items in the dataset are classified using per instance segmentations to assist in accurate localization of items. There are presently two versions of COCO datasets for classified and segmented pictures. The photos in the dataset were collected from everyday scenes offering relevant information. In everyday scenario, many objects or things may be located within the same frame and every item ought to be recognized as a different object and segmented correctly. The COCO dataset contains the naming and segmentation of the items present within the photos. We took this dataset and created our object detection and recognition system for visually impaired people [17].

RESULTS

With OpenCV, we develop our deep learning-based real-time object detector that needs efficient access to our webcam / video stream and application of object detection to each frame. Initially, we have a tendency to capture a frame from the stream and resizing the frame. After that, with the help of DNN module, the frame is converted to a blob. For heavy lifting: set the blob into our Neural Network model as the input and feed the input

through the network that gives us our detections. We've identified objects in the input frame at this point. At that point, we see confidence values and decide if we ought to draw a box and label around the thing. We begin with iteration over our detections, considering that it is possible to identify multiple objects in one image. Always apply a check to the confidence associated with each detection. This confidence value is referred to as probability. When the confidence is high (i.e. above the threshold), the prediction will be displayed in the terminal; a colored bounding box as well as the prediction will be outlined on the image with text.

The model runs smoothly in 4 GB and above RAM operating system. A the end, the model will generate the outputs in various ways such as display in command prompt, in audio mp3 format and in a bounding box with label. At first, the model will generate the output in command prompt which displays the output class label name with location as shown in Fig. 7. The series of output displayed in both frame as well as in command prompt. The frame output is represented in bounding box with class label as shown in Fig. 8. For Fig. 7 and 8, we took screenshots randomly while running the program. Fig. 7 was taken at the beginning of the webcam, Fig. 8 was taken after the camera started adjusting, and finally, Fig. 9 is the correct output. The speech module respectively reads the names of the objects with their position displayed in the command prompt aloud. The speech output is faster with fast internet connection. The voice could be clearly heard with normal speakers as well as the headphones. The accuracy of the object detection module is 90%. Depends on the speed of computer, the final output may process around 6-8 Frames Per second (FPS) and the final output is a deep learning-based object detector.

CONCLUSION

In a wide range of industries, the future of object detection has enormous opportunities. Video processing and object recognition algorithms are proposed based on available resources and dedicated to visually challenged users. People with visual impairments face major challenges when walking around and avoiding obstacles in their daily life. In day-to-day tasks, this program can support visually impaired and blind users. It will lessen the issue of movement and object recognition with a compact solution without the need to bring any additional devices dedicated to it.

Future Scope

Our future work will focus on extending our object detection method to handle more accurate detection technique, HD quality video, projection, scale, angle. We present a platform which utilizes portable cameras, fast HD video link and powerful server to generate 3D sounds. By using advanced new algorithm, the solution could perform accurate real time objective detection with live stream. We will focus on enhancing the object recognition system so that it can better detect and identify objects in extreme and challenging conditions. We will also study the interferences like auditory output and spatial updating of object location.

REFERENCES

1. M. Murad, A. Rehman, A. A. Shah, S. Ullah, M. Fahad and K. M. Yahya, "RFAIDE — An RFID based navigation and object recognition assistant for visually impaired people," 2011 7th International Conference on Emerging Technologies, Islamabad, 2011, pp.1-4. doi: 10.1109/ICET.2011.6048486
2. World Health Organization, "Blindness and Vision Imapirment," World Health Report, Geneva, 2019. https://www.who.int/news-room/fact-sheets/detail/blindness-and-visual-impairment 8 October 2019.
3. K. Matusiak,P. Skulimowski And P.Strumillo, Object recognition in a mobile phone application for visually impaired users, IEEE Trans., 2014.
4. Dionisi, E. Sardini and M. Serpelloni, "Wearable object detection system for the blind," 2012 IEEE International Instrumentation and Measurement Technology Conference Proceedings, Graz, 2012, pp. 1255-1258. doi: 10.1109/I2MTC.2012.6229180

5. Loomis, Jack M.,"Digital map and navigation system for the visually im-paired." Unpublished manuscript, Department of Psychology, University of Cali-fornia, Santa Barbara (1985).
6. Muljowidodo, K., Mochammand A. Rasyid, N. SaptoAdi, and Agus Budiyono."Vision based distance measurement system using single laser pointer design forunderwater vehicle." Indian Journal of Marine science 38, no. 3 (2009): 324-331.
7. R. Gnana Bharathy, "Framework of Object Detection and Classification High Performance Using Video Analytics in Cloud", Published in International Journal of Trend in Scientific Research and Development (ijtsrd), ISSN: 2456-6470, Volume-3 | Issue-1, December 2018, pp.1-8. https://doi.org/10.31142/ijtsrd18906
8. Bari, Neha, Nilesh Kamble, and Parnavi Tamhankar, "Android based object recognition and motion detection to aid visually impaired", International Journal of Advances in Computer Science and Technology, 2014.
9. Jason Yip, Object Detection with Voice Feedback — YOLO v3 + gTTS, https://towardsdatascience.com/object-detection-with-voice-feedback-yolo-v3-gtts-6ec732dca91
10. Samkit Shah, Auto-assistance system for visually impaired person presentation, 2019, page no. 18, https://www.slideshare.net/shahsamkit73/autoassistance-system-for-visually-impaired-person-146004513
11. Joseph Redmon, Santosh Divvala, Ross Girshick , Ali Farhadi, "You Only Look Once: Unified, Real-Time Object Detection," 2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR), Las Vegas, NV, 2016, pp. 779-788, https://arxiv.org/pdf/1506.02640.pdf
12. ODSC – Open Data Science, "Overview of the YOLO Object Detection Algorithm", https://www.medium.com/@ODSC/overview-of-the-yolo-object-detection-algorithm-7b52a745d3e0
13. Redmon, J., Farhadi, A. "YOLO9000: Better, Faster, Stronger." 2017 IEEE Conference on Computer Vision and Pattern Recognition (CVPR) (2016): 6517-6525.
14. gTTS, https://pypi.org/project/gTTS/
15. Lin, Tsung-Yi, Michael Maire, Serge Belongie, James Hays, Pietro Perona, Deva Ramanan, Piotr Dollár, and C. Lawrence Zitnick. "Microsoft coco: Common objects in context." In European conference on computer vision, pp. 740-755. Springer, Cham, 2014.
16. Adrian Rosebrock, "Yolo Object Detection With Opencv," https://www.pyimagesearch.com/2018/11/12/yolo-object-detection-with-opencv/, 2018.
17. Amikelive | Technology Blog, What Object Categories / Labels Are In COCO Dataset?, https://tech.amikelive.com/node-718/what-object-categories-labels-are-in-coco-dataset/, 2018
18. Abdul Vahab, Maruti S Naik, Prasanna G Raikar, Prasad S R, "Applications of Object Detection System," International Research Journal of Engineering and Technology (IRJET) , vol. 6, no. 4, pp. 4186-4192, 2019.
19. Szegedy, C. & Toshev, Alexander & Erhan, Dumitru. (2013). "Deep Neural Networks for object detection", Advances in Neural Information Processing Systems. 26.
20. Redmon, J., & Farhadi, A. (2018). Yolov3: An incremental improvement. arXiv preprint arXiv:1804.02767.

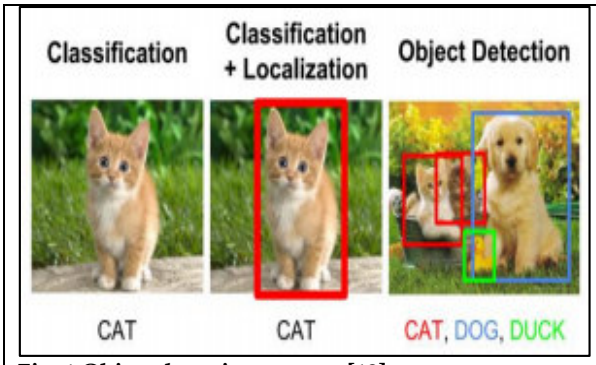

Fig. 1 Object detection process [18]

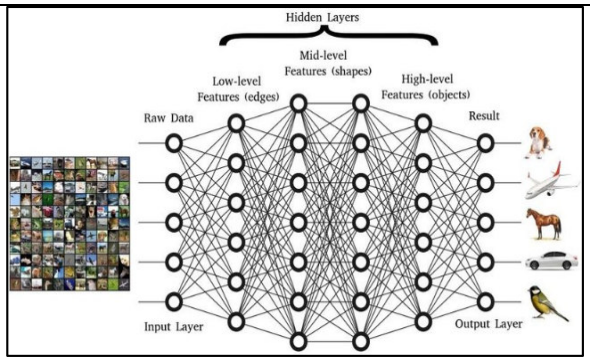

Fig. 2 Basic Working Model of DNNs

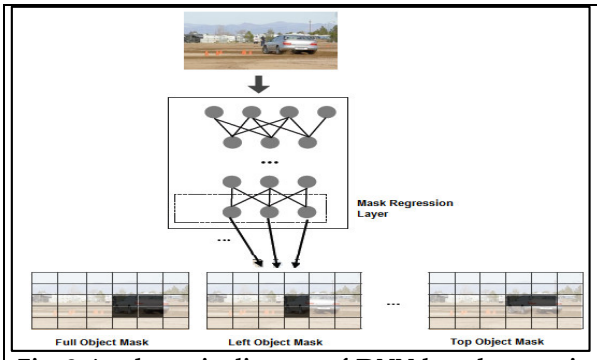

Fig. 3 A schematic diagram of DNN-based regression for object detection [19]

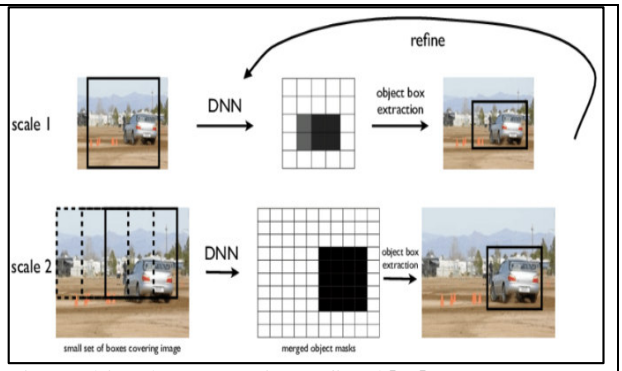

Fig. 4 Object box extraction refined [19]

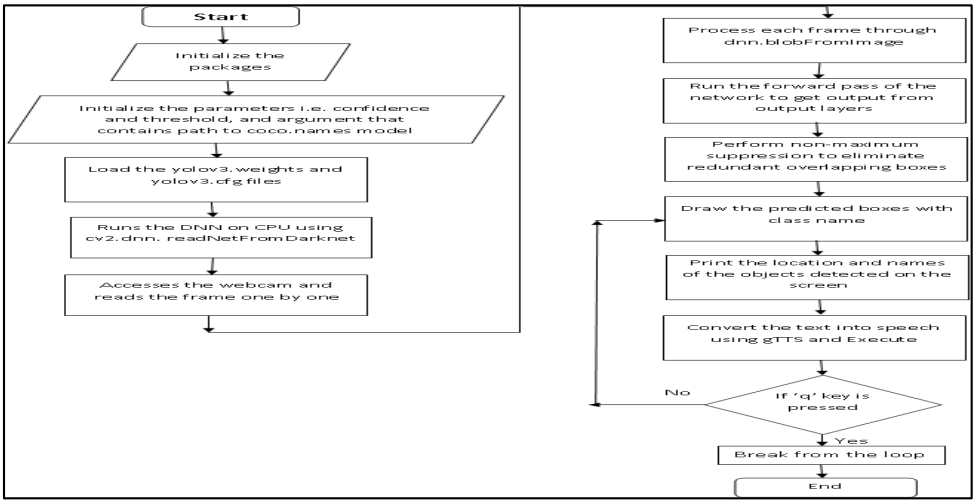

Fig. 5 Flowchart of Real Time Object Recognition using YOLO algorithm

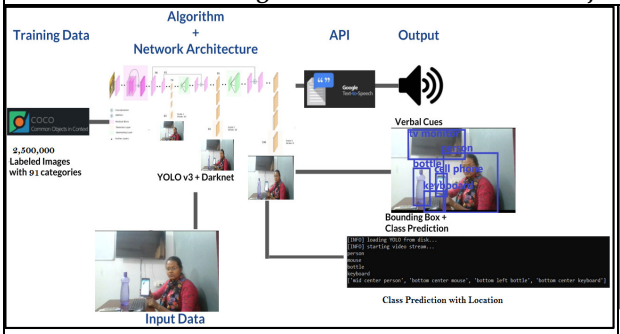

Fig. 6 Proposed Architecture of object detection, object recognition and class prediction with location

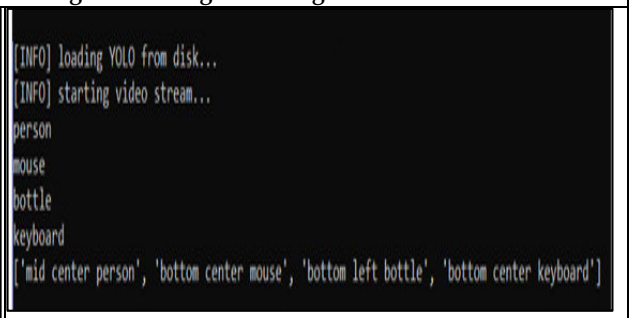

Fig. 7 Snippet of an output generated by our model on first detection

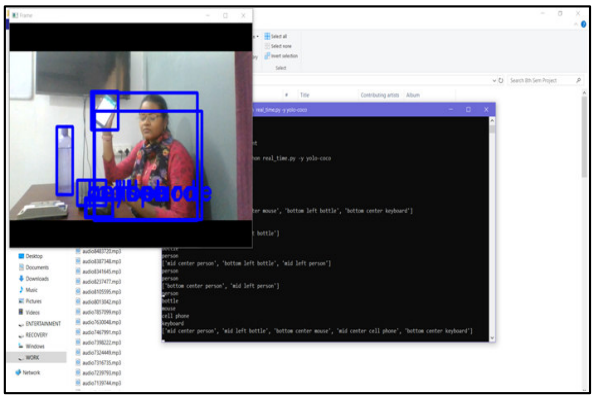

Fig. 8 Output series shown on both Frame and Command Prompt

Fig. 9 Estimated Output with the given Input

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RESEARCH ARTICLE

Analysis of Heavy Metal Ions Extraction from Aqueous Medium Using Different Techniques

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ABSTRACT

Human civilization evolved through industrialization and urbanization as time passed on. This endeavor brought comfort and easiness to the lifestyle of human being. However, this endeavor produces tons of waste materials along with required valuable products. The waste materials contain many chemicals and heavy metals are also part of the byproducts which cannot stopped or avoided. These heavy metal ions due to it's inherent toxicity and non-biodegradable nature accumulate on the living being tissues. This metal ion accumulation causes several diseases among human being and in aquatic animals as well apart from environmental pollution. There are many attempts were made during the last few decades to remove the heavy metal ions and to make the water bodies safe for usage. Here in this manuscript, we have analyzed the range of techniques such as adsorption, phase separation, filtration, etc, that have been employed by various researchers to remove the toxic heavy metal ions. The factors such as pH, adsorbent concentration, adsorbate concentration, temperature, contact time, membrane pore size etc. were also discussed to find out the optimum condition for heavy metal ion removal. Scientists suggested that, adsorption, electronic interaction are playing a major role in metal ion sorption. The experimental results were also compared with theoretical models to have a firsthand knowledge about the type of interactions and the forces responsible for the extraction of heavy metal ions. This work would provide an insight how heavy metal ions could be removed effectively and what are the guiding factors to develop a robust adsorbent for waste water purification.

Keywords: Adsorption, Heavy metal ion, Biomass, membrane filtration, cyclodextrin

INTRODUCTION

Heavy metal ions are the metal ions those are having relatively high density and are considered as toxic to human being and environment. The generally considered heavy metal ions include Copper (Cu), Lead (Pb), Zinc (Zn), Cadmium (Cd), Chromium (Cr), Cobalt (Co), Nickel (Ni), and Iron (Fe)(Atta et al., 2012; Ma et al., 2014; M. Zhang et al., 2019). All of these metal ions are necessary for metabolism, however, upon exceeding the tolerance limit it becomes toxic. One of the major factors associated with these metal ions is, they neither degrade nor excrete easily and accumulate in different parts of the human body leading to toxicity. HMs can generate free radicals leading to oxidative stress and damage to several biological molecules that may result to carcinogenesis and neuro toxicity(Kaewsarn and Yu, 2001; Khalid et al., 2017; Prigione et al., 2009). The HMs could cause both acute and chronic illness to human being depending upon several factors such as the type of HMs, dosage, point of accumulation etc. HMs could affect pulmonary, nervous system, skin, renal etc. causing several diseases such as Neuropathies, Nervous disorder, Skin and respiratory cancer, Pneumoconiosis etc(Ge et al., 2012; Huang et al., 2012; Maan et al., 2016). The HMs also possess serious challenges to aquatic animals for their survival.

There are many sources for the heavy metal ion production such as industry, soil erosion, fertilizer, vehicular emission, paints, and so on. The major concern for heavy metal ion (HM) pollution is the contamination of water bodies such as river, pond, lake etc. by industrial effluents. Although the industrial effluents undergo preliminary treatments for HM ion removal, many times the HM concentration level above the permissible limits were discharged to water bodies. Due to the environmental and Eco toxicity effect of HMs, many researchers have investigated an array of possible solution for the HMs removal from the waste water(Bao et al., 2016; Mahajan and Sud, 2013; Yu et al., 2018). Among the several methodologies, adsorption is the most popular due to the cost effective and efficiency of HMs removal. Here, in this manuscript, other techniques such as membrane filtration, biological methods, usage of deep eutectic solvents, cyclodextrin, hydrogels are also have been discussed for the HMs removal.

RESULTS AND DISCUSSION

Many techniques have been explored by several researchers around the globe to remove HMs from the waste water. Following sections discuss briefly each of the techniques along with the efficiency of techniques.

Using Waste Biomass

Waste biomass is the material derived either from plant origin or animal origin. There are million tons of waste biomass produced worldwide from various sources. The plant biomass includes wood, rice straw, sugar cane bagasse and so on, while the animal waste biomass includes the hard shell of shrimp, crab etc. These waste biomass consists of many chemical components and with progress of time many researchers have explored various applications. Herein, we analyze the application of waste biomass for heavy metal ion adsorption.

(Ngah and Hanafiah, 2008) extensively reviewed the adsorption of heavy metal ions by using different plant waste biomass. They have analyzed the chemical modifications of plant biomass such as rice husk, spent grain, sugarcane bagasse, sawdust, wheat bran, fruit/vegetable waste, weeds, cassava waste, plant fibers, azolla, alfalfa biomass, cottonseed and soybean hulls for heavy metal ion adsorption. Authors have concluded that upon chemical modification using acid and alkali, the adsorption efficiency of waste plant biomass have increased due to increase in active binding site and development of new functional groups. The authors analyzed the adsorption of various heavy metal ions including Cd, Cu, Pb, Zn, Ni and Cr(VI) ions. (Chemistry et al., 2003) investigated the ability of cassava waste biomass (untreated and acid treated) to remove heavy metals (Cu^{2+} and Zn^{2+}) from simulated wastewater. The authors have found that single ion solution shows better ion uptake as compared to double ion solution due to the competitiveness between the ions. While Cu ion uptake was improved upon acid treatment of cassava biomass, there was no appreciable improvement for Zn ion uptake.

(Sekhar et al., 2003) use plant biomass Indian Sarsaparilla for the removal of heavy metal ions. Among the studied metal ions, Pb^{2+} shows highest adsorption as compared to Zn and Cr. Furthermore, Zn, Cr adsorption depends upon the acidic medium of the test solution whereas, Pb metal ion adsorption is independent of pH of the medium. Pb^{2+} ion adsorption is independent of presence of other ions however, Zn^{2+} and Cr^{2+} metal ions adsorption is decreased. Biosorption of heavy metals was investigated by (Chen and Wang, 2008) using waste biomass of brewery. The experimental adsorption data for Pb^{2+}, Ag^{+}, Sr^{2+} and Cs^{+} were fitted well with the Langmuir adsorption isotherm with highest adsorption for lead metal ion. (Singha and Guleria, 2014) have investigated the bioremediation using succinylated waste biomass by varying pH, contact time, temperature and metal ion concentration. Pb^{2+} ion shows highest adsorption as compared to Cd^{2+} followed by Cu^{2+} and Zn^{2+}. The kinetic study reveals that the adsorption is following pseudo-second-order kinetic model whereas, thermodynamic study shows that the adsorption is an exothermic process. (Kaewsarn and Yu, 2001) examined the pre-treated marine biomass of the Padina sp. For the removal of Cd^{2+}. At pH 5, the maximum uptake capacity of 0.53 $mmol.g^{-1}$ was observed.

Using Composite Material

A composite material is something that is made up of two or more individual components and when they are combine, results an enhanced property. There are several ways how a composite could be made and also there are several ways how composite could be used for different applications. There are many literatures that found good results for the application of composite in heavy metal ion removal. (Ravikumar and Udayakumar, 2020) proposed the composite formation from bentonite clay and Moringa oleifera seed. The intercalated nanocomposite was able to extract more than 99 % of Cd^{2+}, Cr^{2+}, and Pb^{2+} ion at pH range of 7-8, 2-3, and 6-7, respectively. (Sheet et al., 2014) prepared nanostructured Graphite Oxide-Silica composite for the removal of heavy metal. They found that although graphite oxide is capable of removing more than 90% of toxic metal ions, the composite made up of Graphite Oxide-Silica in a 3:2 ratios is a better adsorbent for the waste water purification.

(Karnib et al., 2014) prepared activated carbon, silica and silica-activated carbon composite for the removal of heavy metal ion from the simulated water. It has been observed that Ni was most efficiently adsorbed as compared to other investigated heavy metals such as Cd, Pb, and Zn. The adsorption data has been fitted well with the Freundlich isotherm model as suggested from correlation coefficient value. The ion exchange capability of hydroxyapatite was explored by (Choi and Jeong, 2008) in making composite with cellulose. The result shows that the convenient use of hydroxyapatite in the form of composite was able to remove Pb^{2+} heavy metal more efficiently as compared to other heavy metal ions. (Y. Zhang et al., 2019) prepared polypyrrole-chitosan composite electrode for the removal of heavy metal ions from wastewater. The composite was made by chemical polymerization and showed efficient heavy metal ion removal for Cu^{2+} (99.67 mg/g) as compared to other studied metal ions. (Kovin et al., 2016) prepared recycled polymer-natural clay composite for the removal of lead ion from the aqueous solution. The amount of Pb^{2+} ion adsorbed is thrice when the polystyrene is combined with 5 % clay. The absorption capacity increases in the presence of prolonged sunlight.

(Yusuff, 2017) prepared a porous composite based on anthill-chicken eggshell to remove Cu^{2+} and Zn^{2+} ions from aqueous solution by 97.89 % and 99.34 % respectively. The active functional group present on the composite surface is responsible for efficient adsorption. (Fakhre and Ibrahim, 2018) prepared novel supramolecular polysaccharide composite from cellulose and dibenzo-18- crown 6 for heavy meatal ion removal. The composite shows better adsorption towards different ions such as Cd^{2+}, Zn^{2+}, Ni^{2+}, Pb^{2+} and Cu^{2+} as compared to their starting material presumable due to synergistic effect and stable binding as proposed by authors.

Using Nanotechnology

(Dendrimers, 2016) mini review investigated the efficiency of nanomaterials for the removal of toxic metal ions from various literatures and discuss the advantages as well as limitations of these nanomaterials. The advantage with nanomaterial is it's nano size that gives more surface area and active site for adsorption. Dendrimer, silica and chitosan based nano materials were extensively discussed for heavy metal removal. (Kumar and Chawla, 2013)

reviewed the research articles based on nano-metal oxides for the removal of cadmium ion from waste water. This review concludes that zinc oxide, titanium oxide, iron oxide based functionalized nano materials are promising materials for heavy metal ion removal. (Nguyen et al., 2019) studied the adsorption of heavy metal ions such as Pb^{2+}, Ni^{2+} and Cr^{4+} from pharmacy waste water. pH 8 was found to be the optimal condition for the removal of all the studied ions. A new magnetic nanocomposite for the elimination of Hg^{2+} and Pb^{2+} ions from wastewater was synthesized by (Bao et al., 2016). Mercaptoamine-functionalised silica-coated magnetic nanoparticles shows spontaneous as well as endothermic adsorption within studied temperature range.

Magnetic nano porous material was developed by (Vojoudi et al., 2017) for the removal of toxic Hg^{2+}, Pd^{2+}, and Pb^{2+} ions. The material was prepared by using cetyltrimethylammonium bromide (CTAB) surfactant and mesoporous silica through sol-gel technique. Different parameters that could affect the removal efficiency such as pH of the medium, amount of nanomaterial, pollutant concentration, contact time, and so on were investigated and found that under optimal conditions more than 95% of all the heavy metals were extracted. The adsorption-desorption experiment confirms that the nano adsorbent could be used five times without the loss of removal efficiency. Electroplating waste water was investigated for toxic metal ion adsorption by (Hu et al., 2006). The synthesized maghemite nanoparticles were effective for the removal of Cr^{6+}, Cu^{2+}, and Ni^{2+} from wastewater due to electrostatic attraction. The selective metal ion adsorption was highly pH dependent as suggested by authors and the successive adsorption-desorption were carried out successfully.

Using Cyclodextrin

Cyclodextrin (CD) consist of glucose subunits is well studied due to its potential applications in various fields. The hydrophobic interior and hydrophilic exterior makes this molecule suitable as a carrier for several other molecules. Cyclodextrin is used as a drug carrier, complexing agent and so on. The hydroxyl group present in the CD is also explored for adsorption of heavy metal ions by complexing with it. (Badruddoza et al., 2011) impregnated Fe_3O_4 in carboxymethyl-β-cyclodextrin (CM- β-CD) to adsorb Cu^{2+}. The exothermic adsorption attained equilibrium in half an hour of time and the amount is approximately 47.2 mg/g. The desorption of Cu^{2+} was carried out using citric acid and was found to be 96.2 %. The same authors (Zayed et al., 2013) in 2013 investigated adsorption of Pb^{2+}, Cd^{2+}, and Ni^{2+} using the same adsorbent. The multiple COO^- and OH group is responsible for non-competitive removal of toxic metals that follows the order of $Pb^{2+} > > Cd^{2+} > Ni^{2+}$. The experimental adsorption data obey the Langmuir model and pseudo second order kinetics. β-CD combined with graphene oxide to make composite by (Chem et al., 2012) for the removal of Cr^{6+}. The prepared nanocomposite shows excellent removal efficiency of removing 120 mg/g of Cr^{6+} from waste water within one hour.

Nanozerovalent iron nanoparticles were trapped within chitosan-carboxymethyl-β-cyclodextrin complex to make adsorbent beads by (Sikder et al., 2014). The Cr^{6+} and Cu^{2+} heavy metals were extracted by endothermic and exothermic procedure, respectively using the beads. The waste water remediation takes place in two different pathways; one is due to adsorption of heavy metals and the other is due to the reduction of Cr^{6+} to Cr^{3+} and Cu^{2+} to Cu (0) by the oxidation of nanozero iron. The metal ion reduction was established by X-ray photoelectron spectroscopy. (Huang et al., 2015) modified walnut shell biochar using β-cyclodextrin-chitosan composite to prepare a robust adsorbent for Cr^{6+} removal. At pH 2.0, the optimum heavy metal ion removal of 206 mg/g took place endothermically in a spontaneous manner. The modified biochar was found to be more effective (93%) in heavy metal ion removal as compared to virgin biochar (27%). The authors found that the amino and carboxyl groups were responsible for the reduction and complexation of heavy metal ions during removal process.

Using Polymer

(Liu et al., 2010) synthesized a zwitterionic hybrid polymers using pyromellitic acid dianhydride and phenylaminomethyl trimethoxysilane for heavy metal removal. The hybrid material has more than 12 times removal efficiency for Pb^{2+} as compared to Cu^{2+}. The adsorbent can be reused after desorption in HNO_3 solution. (Abdel-halim and Al-deyab, 2011) found that upon modifying sodium alginate with alcoholic HCl, the modified polymer becomes

a robust adsorbent to remove Zn^{2+} from waste water. Different adsorption parameters were investigated by authors and found that at pH 6 maximum adsorption occurs. (Camarillo et al., 2012) prepared polymer surfactant aggregate by using poly diallyldimethylammonium chloride or poly ethylenimine as a support where anionic surfactant is added for complexation and aggregation. The material is used to remove Cr^{3+}, Zn^{2+}, and Cd^{2+} by intermolecular association effectively at a range of pH from 6 to 9. It has also been found that, the aggregate is able to remove heavy metal ions below the critical micelle concentration of surfactants (Shen et al., 2015). This study revealed that polybenzoxazine aerogel was investigated for heavy metal ions removal as a chelating polymer. The authors, (Chaisuwan et al., 2010) found the adsorption capacity in a decreasing order of Sn^{2+} >Cu^{2+} >Fe^{2+} >Pb^{2+} >Ni^{2+} >Cd^{2+} > Cr^{2+}. Furthermore, the experimental data were fitted to Langmuir adsorption model and single ion solution gives better adsorption capability as compared to multi-ion solution adsorption. The metal ion removal efficiency of amidoximated poly (N,N-dipropionitrile acrylamide) powder and amidoximated nonwoven fabric was explored by (Gu, 2004). The result shows the removal trend as follows UO_2^{2+} > Pb^{2+} > Co^{2+} > Cu^{2+} for amidoximated poly (N,N-dipropionitrile acrylamide) and Pb^{2+} > UO_2^{2+} > Co^{2+} > Cu^{2+} for amidoximated nonwoven fabric.

Using Hydrogel

(Wu and Li, 2013) prepared 2-hydroxyethyl acrylate and 2-acrylamido-2-methylpropane sulfonic acid-based hydrogels using gamma radiation for the removal of heavy metal ions. The adsorption efficiency for multi ion solution is Cr^{3+}>Fe^{3+}>Cu^{2+}>Cd^{2+}>Pb^{2+} under optimum pH of 6 and optimum temperature 15 ℃. (Akdemir et al., 2007) synthesize a novel N-vinylpyrrolidone/acrylic acid/2-acrylamido-2-methylpropane sulfonic acid hydrogels by UV-curing technique. The addition of 2-acrylamido-2-methylpropane sulfonic acid decreases thermal stability, however it increases swelling ratio. The synthesized hydrogels were used to adsorb heavy metal ions with a preferential order of Cd^{2+} > Cu^{2+} > Fe^{3+}. (Wu and Li, 2013) prepared poly(Hydroxyethyl methacrylate/Maleamic acid) hydrogel by using gamma radiation. The hydrogels were found to form chelation using -NH_2 group and ion exchange using -COOH group with toxic metal ions. The selectivity order for extraction was found to be in the order of Pb^{2+} > Cu^{2+} > Ni^{2+} > Cd^{2+}. (Atta et al., 2012) synthesize poly-2-acrylamido-2-methylpropanesulfonic acid hydrogels by free radical polymerization. The attraction between metal ion and ionic part of hydrogel is responsible for the heavy metal ions removal with a preferential order of Cd^{2+} > Cu^{2+} > Fe^{3+}. Carboxymethyl cellulose and polyacrylamide based hydrogel was prepared by (Godiya et al., 2018) for the heavy metal ion extraction. The hydrogels were used for the removal of Cu^{2+}, Pb^{2+}, and Cd^{2+} and in case of Cu^{2+} ion, the adsorbed ions were reduced in situ to form nanocomposite hydrogel and subsequently used as catalyst (Ju et al., 2009) studied the removal of Pb^{2+} ions from aqueous solutions using the benzo-18-crown-6-acrylamide and poly(N-isopropylacrylamide) hydrogels. The prepared hydrogels adsorb heavy metal ions below lower critical solution temperature (LCST) and desorb the ion above LCST.

Using Deep Eutectic Solvents

(Chen et al., 2018) prepared a novel magnetic deep eutectic solvents (DES) by combining graphene oxide and DES that composed of choline chloride/itaconic acid/3-mercaptopropionic acid (molar ratio 2:1:1). The prepared sample was used for solid phase extraction in the extraction of heavy metal ion Hg^{2+}. Under optimum condition, 99.9% of heavy metal ion was removed. Further, even after seven cycle of adsorption-desorption, the removal efficiency of adsorbent was above 90%. (Akib et al., 2017) prepared novel adsorbent by combining tetra-n-butyl ammonium bromide and glycerol to make DES that is functionalized with carbon nanotubes. The adsorbent was able to remove the Hg^{2+} ion with an efficiency of 177.76 mg/g and obey Langmuir and Freundlich isotherms models. (Khalid et al., 2016) developed a novel adsorbent for the removal of Pb2+ ion by using choline chloride based DESs those were functionalized with carbon nanotubes. At pH 5, 288.4 mg/g of Pb2+ were removed obeying Langmuir and Freundlich isotherms models. (Fiyadh et al., n.d.) used artificial neural network to describe removal of Hg^{2+} from waste water by functionalizing DES using multi-walled carbon nanotubes. Various parameters such as adsorbent concentration, adsorbate concentration, contact time and pH were investigated for optimum adsorption using different network techniques. The models performance was assessed by different error indicators and correlation coefficient. The nonlinear autoregressive exogenous model was found to be the best model to describe the adsorption performance than the other investigated models.

Using Surfactant and Micelle

(Huang et al., 2010) explored extraction of Cd^{2+} and Zn^{2+} ions from the waste water using sodium dodecyl sulfate surfactant. The heavy metal ions were adsorbed under micellar condition and then the metal ion loaded micelle has undergone ultra-filtration to complete the process. The optimum condition for this process was found to be metal ion concentration of 50 mg/L, surfactant concentration of 2.15 g/L that follow second order kinetics. (Zeftawy and Mulligan, 2011) applied the rhamnolipid biosurfactant for the extraction of Cu^{2+}, Zn^{2+}, Ni^{2+}, Pb^{2+}, and Pb^{2+} from the metal refining industries. The micellar enhance ultrafiltration (MEUF) technique was successfully applied at pH near about 7 and at room temperature. The surfactant to metal ratio was found to be 2:1 for the better heavy metal ion removal. (Ferella et al., 2007) studied municipal waste water remediation of Pb^{2+} and AsO_4^- by MEUF technique. The dodecylbenzenesulfonic acid as anionic surfactant and dodecylamine as cationic surfactant were used for the study with a concentration of 10^{-5} M and 10^{-6} M, respectively. Both the surfactants were used below critical micelle concentration and found to give more than 99% removal of lead and around 19% arsenic from wastewater. (Kim et al., 2008) investigated the removal characteristics of Cd^{2+}, Cu^{2+}, Co^{2+}, and Zn^{2+} ions using sodium dodecyl sulfate (SDS) as an anionic surfactant. Both single metal ion and mixed metal ion removal was explored utilizing MEUF technique. The optimum condition for >95% removal was found to be when surfactant to metal ion ratio was greater than 10. Furthermore, it has been observed that the removal efficiency for single ion extraction was found to be same, however, when multi ions were involved the order of heavy metal ion removal was $Cd^{2+} > Cu^{2+} > Co^{2+}$ Zn^{2+}.

Using Membrane Filtration

(Bessbousse, 2012) fabricated a membrane by combining polyvinyl alcohol and polyethyleneimine for the removal of heavy metals. The membrane was quite stable in water and the removal tendency was $Hg^{2+} > Cu^{2+} > Pb^{2+} > Cd^{2+}$. The experimental metal ion removal capacity was less than theoretical calculation as many internal sites were not exposed to solution phase. (Barakat and Schmidt, 2010) used carboxymethyl cellulose as adsorbent and separated the heavy metal ion- cellulose complex by ultra-filtration. The metal ion removal ability was more in neutral and basic medium as compared to acidic medium and the order of extraction was $Cu^{2+} > Cr^{2+} > Ni^{2+}$. (Ates and Uzal, 2018) studied the aluminum removal from the industrial waste water using membrane filtration. Different types of membrane filtration techniques such as ultrafiltration (UF), nanofiltration (NF), and reverse osmosis (RO) were utilized for Al^{3+} ion removal. It has been found that, both NF and RO shows almost equal removal efficiency with RO technique was having little better efficiency. UF technique being not so efficient in metal ion removal, could be used in pretreatment to improve the life span of NF membrane. (Almasian et al., 2018) prepared polyacrylonitrile /polyaniline -nylon core-shell nanofiber membrane for the removal of Pb^{2+} and Cd^{2+}. The membrane surface was modified by diethylenetriamine and the removal efficiency was found to be 960 and 911 mg/g for Pb^{2+} and Cd^{2+} ions, respectively.

Using Biological Methods

(Alothman et al., 2019) utilized Penicillium chrysogenum and Aspergillus ustus fungi for the bio sorption of Cd^{2+}, Cu^{2+}, and Pb^{2+}. The authors found that the heavy metal ions were extracted by complex combined factors of physical adsorption, ion exchange, complexation, and precipitation methods. (Singh and Gaur, 2007) studied five dried algae for the biosrption of Pb^{2+} and Cu^{2+}. The experimental result shows that Langmuir adsorption model fits better as compared to Freundlich model for the investigated biosorption. Multi metal ion investigation was carried out and found that the extraction efficiency was low if the metal ion concentration increases. (Kapoor and Viraraghavan, 2016) observed that *A. niger* when immobilized on polysulfone, was able to remove 38% Cu^{2+}, 58% Pb^{2+}, and 16% Zn^{2+} ion from waste water by using packed bed column technique. The less removal efficiency of the adsorbent was attributed to the possible deposition of organic materials over the adsorbent eventually leading to less availability of binding site. (Prigione et al., 2009) explored the removal of Cr^{3+} ion from tanning effluent using fungal biomass. *C. elegans* biomass was able to remove up to 40 % of Cr^{3+} heavy metal ion by bio sorption technique. Further it was found that pretreated biomass with NaOH alkali increases the adsorption efficiency. (Akar et al., 2009) found that *Trametes versicolor* and montmorillonite type clay was a good adsorbent for the removal of Cu^{2+} ion. The biosorption

of 62.8 mg/g was obtained at pH 5 and at room temperature. The extraction was confirmed by several experimental techniques and found that both Langmuir and Freundlich model explain the experimental behavior.

CONCLUSION

Here in this manuscript, we have analyzed the range of techniques such as adsorption, phase separation, filtration, biological methods, hydrogels, polymers, deep eutectic solvents etc, that have been employed by various researchers to remove the toxic heavy metal ions. The factors such as pH, adsorbent concentration, adsorbate concentration, temperature, contact time, membrane pore size etc. were also discussed to find out the optimum condition for heavy metal ion removal. Most of the studies suggests that pH is playing a major role in HMs removal. Scientists suggested that, adsorption, electronic interaction are playing a major role in metal ion sorption. The experimental results were also compared with theoretical models to have a firsthand knowledge about the type of interactions and the forces responsible for the extraction of heavy metal ions. Further, single ion and multi ion extraction of HMs were also discussed and found that sometimes multi ion adsorption is less effective as compared to single ion extraction. This work would provide an insight how heavy metal ions could be removed effectively and what are the guiding factors to develop a robust adsorbent for waste water purification.

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REFERENCES

1. Abdel-halim, E.S., Al-deyab, S.S., 2011. Removal of heavy metals from their aqueous solutions through adsorption onto natural polymers. Carbohydr. Polym. 84, 454–458. https://doi.org/10.1016/j.carbpol.2010.12.001
2. Akar, T., Tosun, I., Kaynak, Z., Kavas, E., Incirkus, G., Akar, S.T., 2009. Assessment of the biosorption characteristics of a macro-fungus for the decolorization of Acid Red 44 (AR44) dye. J. Hazard. Mater. 171, 865–871. https://doi.org/10.1016/j.jhazmat.2009.06.085
3. Akdemir, Z.S., Kahraman, M. V, Ko, E., 2007. N -vinylpyrrolidone / acrylic acid / 2-acrylamido-2-methylpropane sulfonic acid based hydrogels□: Synthesis , characterization and their application in the removal of heavy metals 67, 451–460. https://doi.org/10.1016/j.reactfunctpolym.2007.02.007
4. Akib, S., Hashim, M.A., Schwandt, C., 2017. Novel deep eutectic solvent-functionalized carbon nanotubes adsorbent for mercury removal from water. J. Colloid Interface Sci. https://doi.org/10.1016/j.jcis.2017.03.014
5. Almasian, A., Giyahi, M., Fard, G.C., Dehdast, S.A., Maleknia, L., 2018. Removal of Heavy Metal Ions by Modified PAN / PANI-Nylon Core- Shell Nanofibers Membrane□: Filtration Performance , Antifouling and Regeneration Behavior. Chem. Eng. J. https://doi.org/10.1016/j.cej.2018.06.127
6. Alothman, Z.A., Bahkali, A.H., Khiyami, M.A., Alfadul, M., Wabaidur, S.M., Alam, M., Alfarhan, B.Z., 2019. Low cost biosorbents from fungi for heavy metals removal from wastewater. Sep. Sci. Technol. 0, 1–10. https://doi.org/10.1080/01496395.2019.1608242
7. Ates, N., Uzal, N., 2018. Removal of heavy metals from aluminum anodic oxidation wastewaters by membrane filtration.
8. Atta, A.M., Ismail, H.S., Elsaaed, A.M., 2012. Application of Anionic Acrylamide-Based Hydrogels in the Removal of Heavy Metals from Waste Water 123, 2500–2510. https://doi.org/10.1002/app
9. Badruddoza, A.Z.M., Tay, A.S.H., Tan, P.Y., Hidajat, K., Uddin, M.S., 2011. Carboxymethyl- □ -cyclodextrin conjugated magnetic nanoparticles as nano-adsorbents for removal of copper ions□: Synthesis and adsorption studies. J. Hazard. Mater. 185, 1177–1186. https://doi.org/10.1016/j.jhazmat.2010.10.029
10. Bao, S., Li, K., Ning, P., Peng, J., Jin, X., Tang, L., 2016. Highly effective removal of mercury and lead ions from

wastewater by mercaptoamine-functionalised silica-coated magnetic nano-adsorbents: Behaviours and mechanisms. Appl. Surf. Sci. https://doi.org/10.1016/j.apsusc.2016.09.098

11. Barakat, M.A., Schmidt, E., 2010. Polymer-enhanced ultra fi ltration process for heavy metals removal from industrial wastewater. DES 256, 90–93. https://doi.org/10.1016/j.desal.2010.02.008
12. Bessbousse, H., 2012. Characterisation of metal-complexing membranes prepared by the semi-interpenetrating polymer networks technique . Application to the removal of heavy metal ions from aqueous solutions 187, 16–28. https://doi.org/10.1016/j.cej.2011.12.079
13. Camarillo, R., Pérez, Á., Cañizares, P., Lucas, A. De, 2012. Removal of heavy metal ions by polymer enhanced ultra fi ltration Batch process modeling and thermodynamics of complexation reactions. DES 286, 193–199. https://doi.org/10.1016/j.desal.2011.11.021
14. Chaisuwan, T., Komalwanich, T., Luangsukrerk, S., Wongkasemjit, S., 2010. Removal of heavy metals from model wastewater by using polybenzoxazine aerogel. DES 256, 108–114. https://doi.org/10.1016/j.desal.2010.02.005
15. Chem, J.M., Fan, L., Luo, C., Sun, M., Qiu, H., 2012. Synthesis of graphene oxide decorated with magnetic cyclodextrin for fast chromium removal † 24577–24583. https://doi.org/10.1039/c2jm35378d
16. Chemistry, I., Harcourt, P., Box, U.P.O., Harcourt, P., 2003. Removal of Cu (II) and Zn (II) ions from wastewater by cassava (Manihot esculenta Cranz) waste biomass 2, 360–364.
17. Chen, C., Wang, J., 2008. Removal of Pb 2 + , Ag + , Cs + and Sr 2 + from aqueous solution by brewery ' s waste biomass 151, 65–70. https://doi.org/10.1016/j.jhazmat.2007.05.046
18. Chen, J., Wang, Y., Wei, X., Xu, P., Xu, W., Ni, R., Meng, J., 2018. Author ' s Accepted Manuscript. Talanta. https://doi.org/10.1016/j.talanta.2018.06.016
19. Choi, S., Jeong, Y., 2008. The Removal of Heavy Metals in Aqueous Solution by Hydroxyapatite / Cellulose Composite 9, 267–270.
20. Dendrimers, T., 2016. Dendrimers , mesoporous silicas and chitosan-based nanosorbents for the removal of heavy-metal ions□: A Review. Int. J. Biol. Macromol. https://doi.org/10.1016/j.ijbiomac.2016.02.005
21. Fakhre, N.A., Ibrahim, B.M., 2018. The use of new chemically modified cellulose for heavy metal ion adsorption. J. Hazard. Mater. 343, 324–331. https://doi.org/10.1016/j.jhazmat.2017.08.043
22. Ferella, F., Prisciandaro, M., Michelis, I. De, Veglio, F., 2007. Removal of heavy metals by surfactant-enhanced ultrafiltration from wastewaters 207, 125–133. https://doi.org/10.1016/j.desal.2006.07.007
23. Fiyadh, S.S., Alomar, M.K., Zurina, W., Jaafar, B., n.d. Artificial Neural Network Approach for Modelling of Mercury Ions Removal from Water Using Functionalized CNTs with Deep Eutectic Solvent.
24. Ge, F., Li, M., Ye, H., Zhao, B., 2012. Effective removal of heavy metal ions Cd 2 + , Zn 2 + , Pb 2 + , Cu 2 + from aqueous solution by polymer-modified magnetic nanoparticles. J. Hazard. Mater. 211–212, 366–372. https://doi.org/10.1016/j.jhazmat.2011.12.013
25. Godiya, A.C.B., Cheng, X., Li, D., Lu, X., 2018. SC. J. Hazard. Mater. https://doi.org/10.1016/j.jhazmat.2018.09.076
26. Gu, O., 2004. Removal of Concentrated Heavy Metal Ions from Aqueous Solutions Using Polymers with Enriched Amidoxime. https://doi.org/10.1002/app.20616
27. Hu, J., Chen, G., Lo, I.M.C., Asce, M., 2006. Selective Removal of Heavy Metals from Industrial Wastewater Using Maghemite Nanoparticle□: Performance and Mechanisms 709–715.
28. Huang, J., Zeng, G., Zhou, C., Li, X., Shi, L., He, S., 2010. Adsorption of surfactant micelles and Cd 2 + / Zn 2 + in micellar-enhanced ultrafiltration. J. Hazard. Mater. 183, 287–293. https://doi.org/10.1016/j.jhazmat.2010.07.022
29. Huang, X., Liu, Y., Liu, S., Tan, X., Ding, Y., Zeng, G., Zhou, Y., Zhang, M., 2015. RSC Advances chitosan modi fi ed biochars with adsorption / reduction bifuctional roles. RSC Adv. 6, 94–104. https://doi.org/10.1039/C5RA22886G
30. Huang, Z., Liu, S., Zhang, B., Xu, L., Hu, X., 2012. Equilibrium and kinetics studies on the absorption of Cu (II) from the aqueous phase using a ␣ -cyclodextrin-based adsorbent. Carbohydr. Polym. 88, 609–617. https://doi.org/10.1016/j.carbpol.2012.01.009
31. Ju, X., Zhang, S., Zhou, M., Xie, R., Yang, L., Chu, L., 2009. Novel heavy-metal adsorption material□: ion-

recognition P (NIPAM- co -BCAm) hydrogels for removal of lead (II) ions c, 114–118. https://doi.org/10.1016/j.jhazmat.2008.12.089

32. Kaewsarn, P., Yu, Q., 2001. Cadmium (II) removal from aqueous solutions by pre-treated biomass of marine alga Padina sp . 112, 209–213.
33. Kapoor, A., Viraraghavan, T., 2016. Application of immobilized aspergillus niger , biomass in the removal of heavy metals from an industrial wastewater 4529. https://doi.org/10.1080/10934529809376801
34. Karnib, M., Kabbani, A., Holail, H., Olama, Z., 2014. Heavy Metals Removal Using Activated Carbon , Silica and Silica Activated Carbon Composite. Energy Procedia 50, 113–120. https://doi.org/10.1016/j.egypro.2014.06.014
35. Khalid, M., Abdulhakim, M., Hayyan, M., Akib, S., Ibrahim, M., Ali, M., 2017. Chemosphere Allyl triphenyl phosphonium bromide based DES-functionalized carbon nanotubes for the removal of mercury from water. Chemosphere 167, 44–52. https://doi.org/10.1016/j.chemosphere.2016.09.133
36. Khalid, M., Abdulhakim, M., Hayyan, M., Akib, S., Khaleel, R., Ali, M., 2016. Lead removal from water by choline chloride based deep eutectic solvents functionalized carbon nanotubes. J. Mol. Liq. 222, 883–894. https://doi.org/10.1016/j.molliq.2016.07.074
37. Kim, H., Baek, K., Kim, B., Shin, H., Yang, J., 2008. Removal characteristics of metal cations and their mixtures using micellar-enhanced ultrafiltration 25, 253–258.
38. Kovin, T.E.K.I.H., Alsewailem, F.D., Aljlil, S.A., 2016. Recycled polymer / clay composites for heavy-metals adsorption RECYCLED POLYMER / CLAY COMPOSITES FOR HEAVY-METALS ADSORPTION RECIKLIRAN KOMPOZIT POLIMER-GLINA ZA ADSORPCIJO 2–7.
39. Kumar, R., Chawla, J., 2013. Removal of Cadmium Ion from Water / Wastewater by Nano-metal Oxides□: A Review. https://doi.org/10.1007/s12403-013-0100-8
40. Liu, J., Ma, Y., Xu, T., Shao, G., 2010. Preparation of zwitterionic hybrid polymer and its application for the removal of heavy metal ions from water. J. Hazard. Mater. 178, 1021–1029. https://doi.org/10.1016/j.jhazmat.2010.02.041
41. Ma, W., Zong, P., Cheng, Z., Wang, B., Sun, Q., 2014. Adsorption and bio-sorption of nickel ions and reuse for 2-chlorophenol catalytic ozonation oxidation degradation from water. J. Hazard. Mater. 266, 19–25. https://doi.org/10.1016/j.jhazmat.2013.12.007
42. Maan, A., Shatirah, H., Mohd, A., Hashim, A., 2016. Functionalization of CNTs surface with Phosphonuim based deep eutectic solvents for arsenic removal from water. Appl. Surf. Sci. https://doi.org/10.1016/j.apsusc.2016.07.079
43. Mahajan, G., Sud, D., 2013. Journal of Environmental Chemical Engineering Application of ligno-cellulosic waste material for heavy metal ions removal from aqueous solution. Biochem. Pharmacol. 1, 1020–1027. https://doi.org/10.1016/j.jece.2013.08.013
44. Ngah, W.S.W., Hanafiah, M.A.K.M., 2008. Removal of heavy metal ions from wastewater by chemically modified plant wastes as adsorbents□: A review 99, 3935–3948. https://doi.org/10.1016/j.biortech.2007.06.011
45. Nguyen, K.M., Nguyen, B.Q., Nguyen, H.T., Nguyen, H.T.H., 2019. Adsorption of arsenic and heavy metals from solutions by unmodified iron-ore sludge. Appl. Sci. 9. https://doi.org/10.3390/app9040619
46. Prigione, V., Zerlottin, M., Refosco, D., Tigini, V., Anastasi, A., Cristina, G., 2009. Bioresource Technology Chromium removal from a real tanning effluent by autochthonous and allochthonous fungi. Bioresour. Technol. 100, 2770–2776. https://doi.org/10.1016/j.biortech.2009.01.002
47. Ravikumar, K., Udayakumar, J., 2020. Moringa oleifera seed composite a novel material for hazardous heavy metals (Cd , Cr and Pb) removal from aqueous systems 11, 123–138.
48. Sekhar, K.C., Kamala, C.T., Chary, N.S., Anjaneyulu, Y., 2003. Removal of heavy metals using a plant biomass with reference to environmental control 68, 37–45.
49. Sheet, I., Kabbani, A., Holail, H., 2014. Removal of Heavy Metals Using Nanostructured Graphite Oxide , Silica Nanoparticles and Silica / Graphite Oxide Composite. Energy Procedia 50, 130–138. https://doi.org/10.1016/j.egypro.2014.06.016
50. Shen, L., Nguyen, X., Hankins, N.P., 2015. Removal of Heavy Metal Ions from Dilute Aqueous Solutions by Polymer-Surfactant Aggregates: A Novel Effluent Treatment Process. Sep. Purif. Technol.

https://doi.org/10.1016/j.seppur.2015.07.065

51. Sikder, T., Mihara, Y., Islam, S., Saito, T., Tanaka, S., 2014. Preparation and characterization of chitosan – caboxymethyl- b - cyclodextrin entrapped nanozero-valent iron composite for Cu (II) and Cr (IV) removal from wastewater. Chem. Eng. J. 236, 378–387. https://doi.org/10.1016/j.cej.2013.09.093
52. Singh, A., Gaur, Æ.S.K.M.Æ.J.P., 2007. Removal of heavy metals from aqueous solution by common freshwater filamentous algae 1115–1120. https://doi.org/10.1007/s11274-006-9341-z
53. Singha, A.S., Guleria, A., 2014. Engineering in Agriculture , Environment and Food Utility of chemically modi fi ed agricultural waste okra biomass for removal of toxic heavy metal ions from aqueous solution. Eng. Agric. Environ. Food. https://doi.org/10.1016/j.eaef.2014.08.001
54. Vojoudi, H., Badiei, A., Bahar, S., Ziarani, G.M., Faridbod, F., Ganjali, M.R., 2017. A new nano-sorbent for fast and efficient removal of heavy metals from aqueous solutions based on modification of magnetic mesoporous silica nanospheres. J. Magn. Magn. Mater. https://doi.org/10.1016/j.jmmm.2017.05.065
55. Wu, N., Li, Z., 2013. Synthesis and characterization of poly (HEA / MALA) hydrogel and its application in removal of heavy metal ions from water. Chem. Eng. J. 215–216, 894–902. https://doi.org/10.1016/j.cej.2012.11.084
56. Yu, T., Xue, Z., Zhao, X., Chen, W., Mu, T., 2018. Green synthesis of porous β-cyclodextrin polymers for rapid and efficient removal of organic pollutants and heavy metal ions from water. New J. Chem. 42, 16154–16161. https://doi.org/10.1039/c8nj03438a
57. Yusuff, A.S., 2017. Preparation and characterization of composite anthill-chicken eggshell adsorbent: Optimization study on heavy metals adsorption using response surface methodology. J. Environ. Sci. Technol. 10, 120–130. https://doi.org/10.3923/jest.2017.120.130
58. Zayed, A., Badruddoza, M., Bin, Z., Shawon, Z., Wei, T., Daniel, J., Hidajat, K., Shahab, M., 2013. Fe 3 O 4 / cyclodextrin polymer nanocomposites for selective heavy metals removal from industrial wastewater. Carbohydr. Polym. 91, 322–332. https://doi.org/10.1016/j.carbpol.2012.08.030
59. Zeftawy, M.A.M. El, Mulligan, C.N., 2011. Use of rhamnolipid to remove heavy metals from wastewater by micellar-enhanced ultrafiltration (MEUF). Sep. Purif. Technol. 77, 120–127. https://doi.org/10.1016/j.seppur.2010.11.030
60. Zhang, M., Zhu, L., He, C., Xu, X., Duan, Z., Liu, S., Song, M., 2019. Adsorption performance and mechanisms of Pb (II), Cd (II), and Mn (II) removal by a β -cyclodextrin derivative.
61. Zhang, Y., Xue, Q., Li, F., 2019. Removal of heavy metal ions from wastewater by capacitive deionization using polypyrrole / chitosan composite electrode. https://doi.org/10.1177/0263617418822225

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C[C@@H].1OS(=O) OC1(c2ccccc2)c3ccccc3

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was C[C@@H].1OS(=O)OC1(c2ccccc2)c3ccccc3 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that curcumin can block6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value C[C@@H].1OS(=O)OC1(c2ccccc2)c3ccccc3.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value C[C@@H].1OS(=O)OC1(c2ccccc2)c3ccccc3.

REFERENCES

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Table 1. Results of CDocki

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	C[C@@H].1OS(=O)OC1(c2ccccc2)c3ccccc3	2.9590000000000001	18.722000000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(=O)OCCc1scnc1C

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)OCCc1scnc1C.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES valueCC(=O)OCCc1scnc1C.

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Table 1. Results of CDocki

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(=O)OCCc1scnc1C	14.673999999999999	14.110900000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)c1cc(SC#N)c(C)cc1O

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)c1cc(SC#N)c(C)cc1O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCC(C)c1cc(SC#N)c(C)cc1O.

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(C)c1cc(SC#N)c(C)cc1O	17.626000000000001	19.891999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(CN(C(C)C)C(C)C)OCC

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(CN(C(C)C)C(C)C)OCC.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCCOC(CN(C(C)C)C(C)C)OCC.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	CCOC(CN(C(C)C)C(C)C)OCC	10.117000000000001	23.271000000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CCOC(=N)C1CCC(O)CC1

Sanjib Naik*

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2	Pharmacophore	CCOC(=N)c1ccc(O)cc1	11.2568	12.8376

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)NC1CCC(CC1)S(=O)(=O)NC2(CCCCC2)C(=O)O

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CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCC(=O)NC1CCC(CC1)S(=O)(=O)NC2(CCCCC2)C(=O)O.

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2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDocki

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(=O)Nc1ccc(cc1)S(=O)(=O)NC2(CCCCC2)C(=O)O	17.454000000000001	25.277000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of corona byNN1C=CC2CCCCC2C1=N

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was NN1C=CC2CCCCC2C1=N (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NN1C=CC2CCCCC2C1=N.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueNN1C=CC2CCCCC2C1=N.

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Table 1. Results of CDocki

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	NN1C=Cc2ccccc2C1=N	10.086	13.558

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C[C@H].(SCS[C@H].(C)C(=O)O)C(=O)O

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

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CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueC[C@H].(SCS[C@H].(C)C(=O)O)C(=O)O.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	C[C@H].(SCS[C@H].(C)C(=O)O)C(=O)O	21.058	23.495999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(=O)C(N(C)C) C(=O)OCC

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(=O)C(N(C)C)C(=O)OCC.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCCOC(=O)C(N(C)C)C(=O)OCC.

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Table 1. Results of CDocki

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)C(N(C)C)C(=O)OCC	20.774000000000001	24.876999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC(=O)CCC1NCCCN1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC(=O)CCC1NCCCN1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueOC(=O)CCC1NCCCN1.

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Table 1. Results of CDocki

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	OC(=O)CCc1ncccn1	20.605	14.33

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1CC(C)C(CC(=O)O)C(C)C1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	Cc1cc(C)c(CC(=O)O)c(C)c1	20.253	18.794

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by NC1CC(CCC(=O)O) CCC1O

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Keywords: Corona, Virus, Docking, Biovia

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Nc1cc(CCC(=O)O)ccc1O	19.776	17.202999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M enzyme of corona by NS(=O)(=O)C1CC (C(=O) O)C(NCC2CCCCC2)CC1CL

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RESEARCH ARTICLE

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COC(=O)CS[C@H].(C)CC(=O)OC	19.192	19.239000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by NC1CCC2CC3CCC(N)CC3S(=O)(=O)C2C1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was NC1CCC2CC3CCC(N)CC3S(=O)(=O)C2C1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC1CCC2CC3CCC(N)CC3S(=O)(=O)C2C1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueNC1CCC2CC3CCC(N)CC3S(=O)(=O)C2C1.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Nc1ccc2Cc3ccc(N)cc3S(=O)(=O)c2c1	19.055	27.216000000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by COC(=O)C1=CC=COC1=O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was COC(=O)C1=CC=COC1=O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC(=O)C1=CC=COC1=O.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value COC(=O)C1=CC=COC1=O.

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1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	COC(=O)C1=CC=COC1=O	2.3778800000000002	16.9894

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1(C)SC(C)(C)N(C=O)[C@H].1C(=O)O

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1(C)SC(C)(C)N(C=O)[C@H].1C(=O)O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCC1(C)SC(C)(C)N(C=O)[C@H].1C(=O)O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1(C)SC(C)(C)N(C=O)[C@H].1C(=O)O	17.314	19.731999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by O=C1N[C@H]. (CO1) C2CCCCC2

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was O=C1N[C@H].(CO1)C2CCCCC2 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value O=C1N[C@H].(CO1)C2CCCCC2.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueO=C1N[C@H].(CO1)C2CCCCC2.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	O=C1N[C@H].(CO1)c2ccccc2	9.9640000000000004	14.061999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(=O)CNC(C)(C)C

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(=O)CNC(C)(C)C (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(=O)CNC(C)(C)C.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CCOC(=O)CNC(C)(C)C.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)CNC(C)(C)C	17.001000000000001	17.120999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(=N)C1CCC(O)CC1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(=N)C1CCC(O)CC1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(=N)C1CCC(O)CC1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CCOC(=N)C1CCC(O)CC1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOC(=N)c1ccc(O)cc1	18.952000000000002	20.533000000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CN1CCCN2CCCN=C12

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CN1CCCN2CCCN=C12 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN1CCCN2CCCN=C12.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES valueCN1CCCN2CCCN=C12.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CN1CCCN2CCCN=C12	10.460599999999999	14.2866

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC1CC2C[NH2+].[C@@H].(CC2CC1OC)C(=O)O

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ABSTRACT

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC1CC2C[NH2+]. [C@@H].(CC2CC1OC)C(=O)O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value COC1CC2C[NH2+]. [C@@H].(CC2CC1OC)C(=O)O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COc1cc2C[NH2+]. [C@@H].(Cc2cc1OC)C(=O)O	9.7390000000000008	20.699999999999999

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)NC1=NC(=O)NC=C1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CC(=O)NC1=NC(=O)NC=C1.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
3. D. Das, S. Das, M. Pandey, D. Bhattacharyay. "In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis", European Journal of Medicinal Plants (2020) 31(4), 19-24.

Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(=O)NC1=NC(=O)NC=C1	13.408300000000001	16.388400000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1(C)OC(=O)C[C@H].1C(=O)O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC1(C)OC(=O)C[C@H].1C(=O)O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1(C)OC(=O)C[C@H].1C(=O)O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC1(C)OC(=O)C[C@H].1C(=O)O.

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1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
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3. D. Das, S. Das, M. Pandey, D. Bhattacharyay. "In silico Analysis of Phytochemicals from Mucunapruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis", European Journal of Medicinal Plants (2020) 31(4), 19-24.

Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1(C)OC(=O)C[C@H].1C(=O)O	16.539999999999999	18.872

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by ONS(=O)(=O)C1CCCCC1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was ONS(=O)(=O)C1CCCCC1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value ONS(=O)(=O)C1CCCCC1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value ONS(=O)(=O)C1CCCCC1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	ONS(=O)(=O)c1ccccc1	9.375	12.887

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)O[C@@H]. 1CS [C@H].(O1)C(=O)O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(=O)O[C@@H].1CS[C@H].(O1)C(=O)O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)O[C@@H].1CS[C@H].(O1)C(=O)O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCC(=O)O[C@@H].1CS[C@H].(O1)C(=O)O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(=O)O[C@@H].1CS[C@H].(O1)C(=O)O	15.547000000000001	18.376000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)C1=C([O-].)C=C(C)OC1=O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(=O)C1=C([O-].)C=C(C)OC1=O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)C1=C([O-].)C=C(C)OC1=O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC(=O)C1=C([O-].)C=C(C)OC1=O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(=O)C1=C([O-].)C=C(C)OC1=O	15.308	24.129000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCN(CC)CC1CC(N)CCC1O

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCN(CC)CC1CC(N)CCC1O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CCN(CC)CC1CC(N)CCC1O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCN(CC)Cc1cc(N)ccc1O	15.132999999999999	18.428999999999998

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC[C@@H]. (O) COC1CCC(CC2CCC(OC[C@H].(O)CO)CC2)CC1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

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CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC[C@@H].(O)COC1CCC(CC2CCC(OC[C@H].(O)CO)CC2)CC1.

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Table 1. Results of CDock

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	OC[C@@H].(O)COc1ccc(Cc2ccc(OC[C@H].(O)CO)cc2)cc1	15.026	35.726999999999997

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1=CC(=O) OC2CC (OC(=O)C3CCC(NC(=N)N)CC3)CCC12

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1=CC(=O)Oc2cc(OC(=O)c3ccc(NC(=N)N)cc3)ccc12	14.723000000000001	29.385999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C) [C@@H]. 1CC [C@@H].(C)C[C@H].1OC(=O)C(O)O

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)[C@@H].1CC[C@@H].(C)C[C@H].1OC(=O)C(O)O.

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCC(C)[C@@H].1CC[C@@H].(C)C[C@H].1OC(=O)C(O)O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(C)[C@@H].1CC[C@@H].(C)C[C@H].1OC(=O)C(O)O	14.462999999999999	22.033999999999999

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RESEARCH ARTICLE

Deactivation Deactivation of 6M3M Enzyme of Corona by CCOC(=O)[C@@H].1C[NH2+].CCC1=O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(=O)[C@@H].1C[NH2+].CCC1=O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)[C@@H].1C[NH2+].CCC1=O	14.327999999999999	18.943999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)C1CC2CCCCC2C(O)C1O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(=O)C1CC2CCCCC2C(O)C1O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(=O)c1cc2CCCCc2c(O)c1O	14.315	19.010999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC1CC(CC(OC)C1O)C(=O)C

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COc1cc(cc(OC)c1O)C(=O)C	14.038	21.173999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC(=O)[C@@H].1CS [C@@H].(N1)C2CCC(CC2)[C@@H].3N[C@@H].(CS3)C(=O)O

Trupti Mayee Mishra, Supriya Khamari, Soubhagya banta Mishra and Minati Sahu*

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC(=O)CCC(=O)N(NC1CCCCC1)C2CCCCC2

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by N[C@H].(CO)CC1CCCCC1

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC(=O)N1CCC[C@H].1C(O)(C2CCCCC2)C3CCCCC3

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RESEARCH ARTICLE

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC1=CC(=O)NC(=O)N1CC=C.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueNC1=CC(=O)NC(=O)N1CC=C.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	NC1=CC(=O)NC(=O)N1CC=C	9.1750000000000007	15.512

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)OCCC1SCNC1C

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(=O)OCCC1SCNC1C (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(=O)C(=O) N1CCC (CC1)NC(=O)C2CCCCC2

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CCOC(=O)C(=O)N1CCC(CC1)NC(=O)C2CCCCC2.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)C(=O)N1CCC(CC1)NC(=O)C2CCCCC2	8.9960000000000004	28.184999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC1CC([O-].)NC2 CCCCC12

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CC([O-].)NC2CCCCC12.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Oc1cc([O-].)nc2ccccc12	15.962999999999999	26.213000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1(C)CC(CC(C)(C)N1O)C(=O)O

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CN(C)CCS[C@H]. (CO) C1CCCCC1

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1(C)N(O)[C@H].(NC1=S)C2CCCCC2

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)OC(OC (=O) C)C(=C)C

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CN1C(=O)N=C(N)N=C1C(C)(C)C

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CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CN1C(=O)N=C(N)N=C1C(C)(C)C.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CN1C(=O)N=C(N)N=C1C(C)(C)C	7.0579999999999998	18.617000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by NC1CCC2CCCC(O)C2N1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was NC1CCC2CCCC(O)C2N1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC1CCC2CCCC(O)C2N1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value NC1CCC2CCCC(O)C2N1.

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2	Pharmacophore	Nc1ccc2cccc(O)c2n1	7.0069999999999997	16.733000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC1CCCCC1C (=C) N2CCNC2

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ABSTRACT

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CCCCC1C(=C)N2CCNC2.

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC1CCCCC1C(=C)N2CCNC2.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Oc1ccccc1C(=C)n2ccnc2	6.8399999999999999	19.158999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1=NCCC2C1 [NH]. C3CC(O)CCC23

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1=NCCC2C1[NH].C3CC(O)CCC23.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC1=NCCC2C1[NH].C3CC(O)CCC23.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1=NCCc2c1[nH].c3cc(O)ccc23	6.7519999999999998	18.012

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC1CCC2NC(O)CCC2C1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was OC1CCC2NC(O)CCC2C1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CCC2NC(O)CCC2C1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC1CCC2NC(O)CCC2C1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Oc1ccc2nc(O)ccc2c1	6.7290000000000001	14.923

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by NNC(=O)C(=O) NC1CCCCC1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was NNC(=O)C(=O)NC1CCCCC1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NNC(=O)C(=O)NC1CCCCC1.

CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	NNC(=O)C(=O)NC1CCCCC1	6.5119999999999996	16.248999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C1CCN2CCCN=C2CC1

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Keywords: Corona, Virus, Docking, Biovia

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Table 1. Results of CDock

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC1C2C(=O) CCC(=O) C2C(O)C3CCCCC13

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CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Oc1c2C(=O)CCC(=O)c2c(O)c3ccccc13	5.6520000000000001	20.498000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of corona by OC1CCC(NC2CCC3CCCCC3C2)CC1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was OC1CCC(NC2CCC3CCCCC3C2)CC1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1]. A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2]. The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CCC(NC2CCC3CCCCC3C2)CC1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC1CCC(NC2CCC3CCCCC3C2)CC1.

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2	Pharmacophore	Oc1ccc(Nc2ccc3ccccc3c2)cc1	5.6420000000000003	24.687000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCC1=C(O) C2CCCCC2N(C1=O)C3CCCCC3

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCC1=C(O)C2CCCCC2N(C1=O)C3CCCCC3.

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCCC1=C(O)C2CCCCC2N(C1=O)C3CCCCC3.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	CCC1=C(O)c2ccccc2N(C1=O)c3ccccc3	5.617	27.391999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1=NN[C@H].(C1) C2CCC(O)CC2

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1=NN[C@H].(C1)C2CCC(O)CC2.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCC1=NN[C@H].(C1)C2CCC(O)CC2.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1=NN[C@H].(C1)c2ccc(O)cc2	5.3739999999999997	15.843

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by O=C1CCCCCN1SSN2CCCCCC2=O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was O=C1CCCCCN1SSN2CCCCCC2=O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value O=C1CCCCCN1SSN2CCCCCC2=O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueO=C1CCCCCN1SSN2CCCCCC2=O.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	O=C1CCCCCN1SSN2CCCCCC2=O	5.3520000000000003	18.841999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC1CCC(\C=C\C)CC1O

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOc1ccc(\C=C\C)cc1O	4.6050000000000004	19.077999999999999

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC1CCC2[NH].C(NC2C1)S(=O)CC3NCC(C)C(OC)C3C

Milan Pradhan and Swapna Meher*

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing"Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was COC1CCC2[NH].C(NC2C1)S(=O)CC3NCC(C)C(OC)C3C (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC1CCC2[NH].C(NC2C1)S(=O)CC3NCC(C)C(OC)C3C.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value COC1CCC2[NH].C(NC2C1)S(=O)CC3NCC(C)C(OC)C3C.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"-C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COc1ccc2[nH].c(nc2c1)S(=O)Cc3ncc(C)c(OC)c3C	3.694	23.893000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1OC(C[N+].(C)(C)C)CC1

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Keywords: Corona, Virus, Docking, Biovia

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC1OC(C[N+].(C)(C)C)CC1.

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Table 1. Results of CDock

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Cc1oc(C[N+].(C)(C)C)cc1	3.6549999999999998	5.9020000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCC1(C)[C@H].(C#N)C(=O)NC(=O)[C@H].1C#N

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Keywords: Corona, Virus, Docking, Biovia

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"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people [1].A new species of corona named as "COVID-19"caused this attack. The issue is that there is no drug discovered [2].The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCC1(C)[C@H].(C#N)C(=O)NC(=O)[C@H].1C#N.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES valueCCC1(C)[C@H].(C#N)C(=O)NC(=O)[C@H].1C#N.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCC1(C)[C@H].(C#N)C(=O)NC(=O)[C@H].1C#N	3.3029999999999999	17.648

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Biovia

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1(C)CC(O)CC(C)(C)N1O	3.2509999999999999	17.391999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC(=O)C[C@@].12C [C@H].3C[C@@H].(C1)C[C@].(C3)(C2)C(=O)O

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	OC(=O)C[C@@].12C[C@H].3C[C@@H].(C1)C[C@].(C3)(C2)C(=O)O	3.1440000000000001	28.532

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C[C@H].1C[C@H].(CC(C)(C)C1)OC=O

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value C[C@H].1C[C@H].(CC(C)(C)C1)OC=O.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value C[C@H].1C[C@H].(CC(C)(C)C1)OC=O.

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2	Pharmacophore	C[C@H].1C[C@H].(CC(C)(C)C1)OC=O	8.7360000000000007	16.960000000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by OC1CCC2NC(O)CCC2C1

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CCC2NC(O)CCC2C1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value OC1CCC2NC(O)CCC2C1.

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Table 1. Results of CDock

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	Oc1ccc2nc(O)ccc2c1	2.4030200000000002	10.498100000000001

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Biovia

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Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1C2C(=O)CCC(=O)C2C(O)C3CCCCC13.

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The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value OC1C2C(=O)CCC(=O)C2C(O)C3CCCCC13.

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2	Pharmacophore	Oc1c2C(=O)CCC(=O)c2c(O)c3ccccc13	1.21922	16.3188

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RESEARCH ARTICLE

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2	Pharmacophore	CC(=O)O[C@@H].1CS[C@H].(O1)C(=O)O	11.7799	13.8301

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC1(C)COC(OC1)C2 CCNCC2

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Received: 24 Mar 2020 Revised: 25 Apr 2020 Accepted: 26 May 2020

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2	Pharmacophore	CC1(C)COC(OC1)C2CCNCC2	1.0941099999999999	17.245799999999999

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RESEARCH ARTICLE

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2	Pharmacophore	NN1C=Cc2ccccc2C1=N	11.6211	14.459

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RESEARCH ARTICLE

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2	Pharmacophore	CC1(C)SC(C)(C)N(C=O)[C@H].1C(=O)O	12.0906	16.035699999999999

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	Cc1ccc(O)c(c1)C(=O)NO	12.738099999999999	16.428000000000001

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RESEARCH ARTICLE

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by OC(=O)CSCC1CCCC2CCCCC12

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(=O)CC1C(C)[NH].C2CCC(CC12)C(C)C.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CCOC(=O)CC1C(C)[NH].C2CCC(CC12)C(C)C.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)Cc1c(C)[nH].c2ccc(cc12)C(C)C	25.144600000000001	22.204899999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by O=C1CCCCCN1SSN2CCCCCC2=O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was O=C1CCCCCN1SSN2CCCCCC2=O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1]. A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2]. The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value O=C1CCCCCN1SSN2CCCCCC2=O.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value O=C1CCCCCN1SSN2CCCCCC2=O.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	O=C1CCCCCN1SSN2CCCCCC2=O	13.309900000000001	23.0151

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CSC[C@H].(O)CN1N=C(O)C(=C(CL)C1=O)CL

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CSC[C@H].(O)CN1N=C(O)C(=C(CL)C1=O)CL.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CSC[C@H].(O)CN1N=C(O)C(=C(CL)C1=O)CL.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CSC[C@H].(O)CN1N=C(O)C(=C(Cl)C1=O)Cl	8.0209799999999998	17.4892

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CCOC1CCC(\C=C\C) CC1O

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC1CCC(\C=C\C)CC1O.

CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CCOc1ccc(\C=C\C)cc1O	5.0757000000000003	17.1967

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(C)(C)C1CC2C(=O)CC(C)(C)OC2C(O)C1O

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(C)(C)c1cc2C(=O)CC(C)(C)Oc2c(O)c1O	11.0702	14.448499999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C[C@@H].1CN=C (NC2CCCCC2)S1

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RESULTS AND DISCUSSION

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CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	C[C@@H].1CN=C(NC2CCCCC2)S1	2.7069999999999999	16.603000000000002

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)O[C@@H].1C=CC[C@H].2[C@@H].1C(=O)C3C(O)CCCC3C2=O

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C\C=C\[C@H].(OC(=O) C1CCCCC1C(=O)O)C#C

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1(C)COC(OC1)C2 CCNCC2

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1(C)COC(OC1)C2CCNCC2.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC1(C)COC(OC1)C2CCNCC2.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1(C)COC(OC1)C2CCNCC2	2.8639999999999999	16.739999999999998

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(=O)[C@H].1CC[N@@H+].(CC2CCCCC2)CC1=O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(=O)[C@H].1CC[N@@H+].(CC2CCCCC2)CC1=O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CCOC(=O)[C@H].1CC[N@@H+].(CC2CCCCC2)CC1=O.

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)[C@H].1CC[N@@H+].(Cc2ccccc2)CC1=O	2.5219999999999998	11.685

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC1CC(N)C2NCCC C2C1

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC1CC(N)C2NCCCC2C1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value COC1CC(N)C2NCCCC2C1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	COc1cc(N)c2ncccc2c1	2.7400000000000002	14.835000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CON1[C@@H].2CCCC [C@@H].2N(OC)C(=O)C1=O

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CON1[C@@H].2CCCC[C@@H].2N(OC)C(=O)C1=O.

CONCLUSIONS

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CON1[C@@H].2CCCC[C@@H].2N(OC)C(=O)C1=O	2.907	20.318999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC1C(CN2CCCCC2)CCC3CCCCC13

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Keywords: Corona, Virus, Docking, Biovia

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CONCLUSIONS

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Oc1c(CN2CCCCC2)ccc3ccccc13	2.6349999999999998	21.465

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(C)C1CC(SC#N)C(C)CC1O

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Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)C1CC(SC#N)C(C)CC1O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(C)c1cc(SC#N)c(C)cc1O	13.756399999999999	16.954699999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC1CC(C)C(CC(=O)O)C(C)C1

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2	Pharmacophore	Cc1cc(C)c(CC(=O)O)c(C)c1	16.407900000000001	16.5974

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CN1CNC(C(=O)O)C1C(=O)O.

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1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
3. D. Das, S. Das, M. Pandey, D. Bhattacharyay. "In silico Analysis of Phytochemicals from Mucuna pruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis", European Journal of Medicinal Plants (2020) 31(4), 19-24.

Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	Cn1cnc(C(=O)O)c1C(=O)O	13.568300000000001	16.052600000000002

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CCOC(=O)[C@@H].1C [NH2+].CCC1=O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(=O)[C@@H].1C[NH2+].CCC1=O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1]. A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2]. The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(=O)[C@@H].1C[NH2+].CCC1=O.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CCOC(=O)[C@@H].1C[NH2+].CCC1=O.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)[C@@H].1C[NH2+].CCC1=O	19.779800000000002	22.554500000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by C[NH2+]CC(=O)C1CCC(O)C(O)C1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was C[NH2+]CC(=O)C1CCC(O)C(O)C1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value C[NH2+]CC(=O)C1CCC(O)C(O)C1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value C[NH2+]CC(=O)C1CCC(O)C(O)C1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	C[NH2+]CC(=O)c1ccc(O)c(O)c1	27.058499999999999	26.2057

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by COC1CCC2[NH]C(CL)NC2C1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was COC1CCC2[NH]C(CL)NC2C1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC1CCC2[NH]C(CL)NC2C1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value COC1CCC2[NH]C(CL)NC2C1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	COc1ccc2[nH]c(Cl)nc2c1	6.4662800000000002	14.406599999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by C1CCN2CCCN=C2CC1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was C1CCN2CCCN=C2CC1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value C1CCN2CCCN=C2CC1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value C1CCN2CCCN=C2CC1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	C1CCN2CCCN=C2CC1	7.4638499999999999	13.446899999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by NC(=S)NC1CCCCC1O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was NC(=S)NC1CCCCC1O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC(=S)NC1CCCCC1O.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value NC(=S)NC1CCCCC1O.

REFERENCES

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2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
3. D. Das, S. Das, M. Pandey, D. Bhattacharyay. "In silico Analysis of Phytochemicals from Mucuna pruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis", European Journal of Medicinal Plants (2020) 31(4), 19-24.

Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	NC(=S)Nc1ccccc1O	12.044499999999999	14.3904

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by OC1CC([O-])NC2CCCCC12

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was OC1CC([O-])NC2CCCCC12 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CC([O-])NC2CCCCC12.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value OC1CC([O-])NC2CCCCC12.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	Oc1cc([O-])nc2ccccc12	13.318899999999999	24.162299999999998

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RESEARCH ARTICLE

Deactivation Deactivation of 6M3M Enzyme of Corona by CC(=O)CCC1C(C)C(OC(=O)C)C(C)C(C)C1OC(=O)C

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(=O)CCC1C(C)C(OC(=O)C)C(C)C(C)C1OC(=O)C (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)CCC1C(C)C(OC(=O)C)C(C)C(C)C1OC(=O)C.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC(=O)CCC1C(C)C(OC(=O)C)C(C)C(C)C1OC(=O)C.

REFERENCES

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2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(=O)CCc1c(C)c(OC(=O)C)c(C)c(C)c1OC(=O)C	36.651000000000003	32.573999999999998

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RESEARCH ARTICLE

Deactivation Deactivation of 6M03 Enzyme of Corona by COC1CC (CL)CCC1O

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC1CC (CL)CCC1O.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value COC1CC (CL)CCC1O.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	COc1cc(Cl)ccc1O	7.4210000000000003	11.0421

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by COC(=O)[C@@H]1[C@H](C)CC(=CC1=O)O

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was COC(=O)[C@@H]1[C@H](C)CC(=CC1=O)O (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC(=O)[C@@H]1[C@H](C)CC(=CC1=O)O.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value COC(=O)[C@@H]1[C@H](C)CC(=CC1=O)O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	COC(=O)[C@@H]1[C@H](C)CC(=CC1=O)O	8.1698900000000005	19.488199999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by OC(=O)C[NH2+]CC1 CCCCC1

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC(=O)C[NH2+]CC1CCCCC1.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	OC(=O)C[NH2+]Cc1ccccc1	22.277699999999999	19.150200000000002

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(C)(C)[C@H](NC=O) C(=O)O

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)(C)[C@H](NC=O)C(=O)O.

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2	Pharmacophore	CC(C)(C)[C@H](NC=O)C(=O)O	12.976800000000001	13.882400000000001

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RESEARCH ARTICLE

Deactivation Deactivation of 6M03 Enzyme of Corona by C1CCN2CCC [NH+]=C2CC1

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	C1CCN2CCC[NH+]=C2CC1	5.3287000000000004	14.9916

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(C)[C@@H]1CC[C@@H](C)C[C@H]1OC(=O)C(O)O

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	CC(C)[C@@H]1CC[C@@H](C)C[C@H]1OC(=O)C(O)O	9.5355000000000008	24.401800000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by COC1CC (CN2CNNN2) CCC1O

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Keywords: Corona, Virus, Docking, Biovia

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	COc1cc(Cn2cnnn2)ccc1O	3.4635600000000002	18.704799999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(=O)NC(NC(=O)C)C(=O)C1CCCCC1

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RESEARCH ARTICLE

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2	Pharmacophore	OC(=O)CCC(=O)N(Nc1ccccc1)c2ccccc2	14.3324	23.0579

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1OC(C[N+](C)(C)C)CC1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CC1OC(C[N+](C)(C)C)CC1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	Cc1oc(C[N+](C)(C)C)cc1	10.638199999999999	13.2706

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CCC1(C)[C@H](C#N) C(=O)NC(=O)[C@H]1C#N

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCC1(C)[C@H](C#N)C(=O)NC(=O)[C@H]1C#N (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCC1(C)[C@H](C#N)C(=O)NC(=O)[C@H]1C#N.

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CCC1(C)[C@H](C#N)C(=O)NC (=O)[C@H]1C#N	3.3948100000000001	17.149999999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(=O)C1CC2CCCCC2C(O)C1O

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	CC(=O)c1cc2CCCCc2c(O)c1O	9.5921500000000002	17.167000000000002

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RESEARCH ARTICLE

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2	Pharmacophore	CN(C)C[C@H](O)COCc1occc1	11.34	20.551600000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by C[C@H]1C[C@H](CC(C)(C)C1)OC=O1

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2	Pharmacophore	C[C@H]1C[C@H](CC(C)(C)C1)OC=O	9.3759700000000006	15.673

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by C[C@@H]1CC(C)(C)N(CCO)C2CC(C)CCC121

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Keywords: Corona, Virus, Docking, Biovia

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	C[C@@H]1CC(C)(C)N(CCO)c2cc(C)ccc12	11.993499999999999	18.635999999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by NNC(=O)C(=O)NC1 CCCCC11

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Keywords: Corona, Virus, Docking, Biovia

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CONCLUSIONS

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	NNC(=O)C(=O)NC1CCCCC1	8.4795800000000003	21.247800000000002

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by C=CCN1CCS(=O) (=O)CC11

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The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CCOC(=O)CNC(C)(C)C1.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)CNC(C)(C)C	11.790900000000001	15.088699999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by COC(=O)CS[C@H](C)CC (=O)OC1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was COC(=O)CS[C@H](C)CC(=O)OC1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC(=O)CS[C@H](C)CC(=O)OC1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value COC(=O)CS[C@H](C)CC(=O)OC1.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	COC(=O)CS[C@H](C)CC(=O)OC	21.859500000000001	22.578800000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by COC(=O)[C@H]1SCC (=O)[C@H]1C(=O)OC1

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC(=O)[C@H]1SCC(=O)[C@H]1C(=O)OC1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	COC(=O)[C@H]1SCC(=O)[C@H]1C(=O)OC	12.704700000000001	13.642300000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by OC1CC2CCN=CC2CC1O1

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CC2CCN=CC2CC1O1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value OC1CC2CCN=CC2CC1O1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	Oc1cc2CCN=Cc2cc1O	4.50509	7.2308899999999996

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CLC1NC(CL)NC(N1) N2CCCC3CCCCC231

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CLC1NC(CL)NC(N1)N2CCCC3CCCCC231 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CLC1NC(CL)NC(N1)N2CCCC3CCCCC231.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CLC1NC(CL)NC(N1)N2CCCC3CCCCC231.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Quercetin	11.1966	13.2172
2	Pharmacophore	Clc1nc(Cl)nc(n1)N2CCCc3ccccc23	27.039999999999999	19.360099999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1(C)O[C@@H](CC(=O)O)C(=O)O11

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC1(C)O[C@@H](CC(=O)O)C(=O)O11 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1(C)O[C@@H](CC(=O)O)C(=O)O11.

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC1(C)O[C@@H](CC(=O)O)C(=O)O11.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1(C)O[C@@H](CC(=O)O)C(=O)O1	22.975000000000001	22.257999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(=O)[C@](C) (OC(=O) C)C(=O)C1

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

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2	Pharmacophore	CCOC(=O)[C@](C)(OC(=O)C)C(=O)C	22.692	21.198

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)C(=O)OC[C@H](C)C1CCCCC11

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	CC(C)C(=O)OC[C@H](C)c1ccccc1	22.518000000000001	20.922000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC(=O)[C@](C)(N) CC1CCC(O)CC11

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COC(=O)[C@](C)(N)Cc1ccc(O)cc1	22.047999999999998	20.030999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)(C)\C(=C/C(=O)C(C)(C)C)\[O-]1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(C)(C)\C(=C/C(=O)C(C)(C)C)\[O-]1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)(C)\C(=C/C(=O)C(C)(C)C)\[O-]1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC(C)(C)\C(=C/C(=O)C(C)(C)C)\[O-]1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(C)(C)\C(=C/C(=O)C(C)(C)C)\[O-]	21.518999999999998	28.184999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC[C@H](CC1CCCC(O)C1)[C@H](CO)CC2CCCC(O)C21

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC[C@H](CC1CCCC(O)C1)[C@H](CO)CC2CCCC(O)C21.

CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	OC[C@H](Cc1cccc(O)c1)[C@H](CO)Cc2cccc(O)c2	21.065000000000001	34.018999999999998

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)(C)C1CC2C(=O)CC(C)(C)OC2C(O)C1O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC(C)(C)C1CC2C(=O)CC(C)(C)OC2C(O)C1O1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(C)(C)c1cc2C(=O)CC(C)(C)Oc2c(O)c1O	23.129000000000001	24.876999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(=O)CC1C(C)[NH]C2CCC(CC12)C(C)C1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(=O)CC1C(C)[NH]C2CCC(CC12)C(C)C1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(=O)CC1C(C)[NH]C2CCC(CC12)C(C)C1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CCOC(=O)CC1C(C)[NH]C2CCC(CC12)C(C)C1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)Cc1c(C)[nH]c2ccc(cc12)C(C)C	31.315999999999999	29.204000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CLC1NC(CL)NC(N1) N2CCCC3CCCCC231

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CLC1NC(CL)NC(N1)N2CCCC3CCCCC231 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CLC1NC(CL)NC(N1)N2CCCC3CCCCC231.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CLC1NC(CL)NC(N1)N2CCCC3CCCCC231.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Clc1nc(Cl)nc(n1)N2CCCc3ccccc23	30.369	23.620999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)NC(NC(=O)C)C (=O)C1CCCCC11

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)NC(NC(=O)C)C(=O)C1CCCCC11.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC(=O)NC(NC(=O)C)C(=O)C1CCCCC11.

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC(=O)[C@H]1SCC (=O)[C@H]1C(=O)OC1

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)COC(=O)OCC (C)C1

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2	Pharmacophore	CC(C)COC(=O)OCC(C)C	23.989999999999998	19.713000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC(=O)CCCC1CCC(CC1)C(=O)C2CCCCC2C(=O)O1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was OC(=O)CCCC1CCC(CC1)C(=O)C2CCCCC2C(=O)O1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC(=O)CCCC1CCC(CC1)C(=O)C2CCCCC2C(=O)O1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC(=O)CCCC1CCC(CC1)C(=O)C2CCCCC2C(=O)O1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	OC(=O)CCCc1ccc(cc1)C(=O)c2ccccc2C(=O)O	23.727	28.427

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RESEARCH ARTICLE

Deactivation of 6M3M enzyme of corona by CCC1C(C(=O)OC)C2CC(O)CCC2N1CC3CCCCC31

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Keywords: Corona, Virus, Docking, Biovia

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Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCC1C(C(=O)OC)C2CC(O)CCC2N1CC3CCCCC31.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CCC1C(C(=O)OC)C2CC(O)CCC2N1CC3CCCCC31.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCc1c(C(=O)OC)c2cc(O)ccc2n1Cc3ccccc3	23.338000000000001	29.628

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC1CCC2[NH]C(CL)NC2C11

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC1CCC2[NH]C(CL)NC2C11.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value COC1CCC2[NH]C(CL)NC2C11.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COc1ccc2[nH]c(Cl)nc2c1	8.6140000000000008	15.127000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC1CCC(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)CC11

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was COC1CCC(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)CC11 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC1CCC(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)CC11.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value COC1CCC(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)CC11.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COc1ccc(C[C@@H]2NC[C@@H](O)[C@@H]2OC(=O)C)cc1	8.5830000000000002	26.966999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1CCC(CC1)S(=O)(=O)[N-]CL1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Cc1ccc(cc1)S(=O)(=O)[N-]Cl	8.5500000000000007	13.784000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C=CCN1CCS(=O)(=O)CC11

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	C=CCN1CCS(=O)(=O)CC1	8.5009999999999994	16.172000000000001

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RESEARCH ARTICLE

Deactivation Deactivation of 6M3M Enzyme of Corona by COC1CC (CL)CCC1O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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CONCLUSIONS

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Table 1. Results of CDock

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COc1cc(Cl)ccc1O	8.4760000000000009	11.837

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by NC1CCC(NC2CCCCC2)CC11

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC1CCC(NC2CCCCC2)CC11.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value NC1CCC(NC2CCCCC2)CC11.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Nc1ccc(Nc2ccccc2)cc1	7.9269999999999996	14.083

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1=CC(=O)NC2CC(N)CCC121

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC1=CC(=O)NC2CC(N)CCC121 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1=CC(=O)NC2CC(N)CCC121.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC1=CC(=O)NC2CC(N)CCC121.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1=CC(=O)Nc2cc(N)ccc12	7.8739999999999997	16.178000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C[NH2+]CC(=O)C1CCC(O)C(O)C11

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value C[NH2+]CC(=O)C1CCC(O)C(O)C11.

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2	Pharmacophore	C[NH2+]CC(=O)c1ccc(O)c(O)c1	7.8159999999999998	6.6989999999999998

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)N(CC[C@](C(=O)N)(C1CCCCC1)C2CCCCN2)C(C)C1

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	CC(C)N(CC[C@](C(=O)N)(c1ccccc1) c2ccccn2)C(C)C	7.718	33.409999999999997

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)C[C@H]1S[C@H](C)C(=N1)C1

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Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)C[C@H]1S[C@H](C)C(=N1)C1.

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2	Pharmacophore	CC(C)C[C@H]1S[C@H](C)C(=N1)C	7.4169999999999998	13.949

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C[C@H](O)C\C=N\C1 CCCC2CCCCC121

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC(=O)[C@@H]1[C@H](C)CC(=CC1=O)O1

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(=O)NC1=NC(=O) NC=C11

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CN1CNC(C(=O)O)C1C (=O)O1

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RESEARCH ARTICLE

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN1CCCN2CCCN=C121.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CN1CCCN2CCCN=C121.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CN1CCCN2CCCN=C12	11.43	14.731999999999999

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RESEARCH ARTICLE

Deactivation Deactivation of 6M3M Enzyme of Corona by CC1(C)CC(CC(C)(C)N1O) OC(=O)C2CCCCC21

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC1(C)CC(CC(C)(C)N1O)OC(=O)C2CCCCC21 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1(C)CC(CC(C)(C)N1O)OC(=O)C2CCCCC21.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC1(C)CC(CC(C)(C)N1O)OC(=O)C2CCCCC21.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC1(C)CC(CC(C)(C)N1O)OC(=O)c2ccccc2	11.416	23.914999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCC(=O)OC1SC (NCCC2CCCCC2)[N+](C)C1C1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCC(=O)OC1SC(NCCC2CCCCC2)[N+](C)C1C1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CCC(=O)OC1SC(NCCC2CCCCC2)[N+](C)C1C1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCC(=O)Oc1sc(NCCc2ccccc2)[n+](C)c1C	10.957000000000001	15.875999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC(=O)C[NH2+]CC1 CCCCC11

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC(=O)C[NH2+]CC1CCCCC11.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC(=O)C[NH2+]CC1CCCCC11.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	OC(=O)C[NH2+]Cc1ccccc1	10.923	9.3770000000000007

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by NC(=S)NC1CCCCC1O1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was NC(=S)NC1CCCCC1O1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC(=S)NC1CCCCC1O1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	NC(=S)Nc1ccccc1O	10.816000000000001	15.718

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CCOC(=O)C(=C (C1CCCCC1)C2CCCCC2)CC(=O)O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)C(=C(c1ccccc1)c2ccccc2)CC(=O)O	10.779999999999999	30.25

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CSC[C@H](O)CN1N=C(O)C(=C(CL)C1=O)CL1

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)C1=CC(=O)OC2C3 CCCN4CCCC(CC12)C341

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2	Pharmacophore	CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34	10.265000000000001	24.181999999999999

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC1CCC(C)N1CC2CCNCC21

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CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CC1CCC(C)N1CC2CCNCC21.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Cc1ccc(C)n1CC2CCNCC2	13.709	20.202000000000002

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC(=O)C1[NH]C(C(=O)O)C2OCCOC121

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was OC(=O)C1[NH]C(C(=O)O)C2OCCOC121 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC(=O)C1[NH]C(C(=O)O)C2OCCOC121.

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC(=O)C1[NH]C(C(=O)O)C2OCCOC121.

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	OC(=O)c1[nH]c(C(=O)O)c2OCCOc12	13.535	15.541

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)(C)[C@H](NC=O)C(=O)O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC1CC2CCN=CC2C C1O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC1CC2CCN=CC2CC1O1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Oc1cc2CCN=Cc2cc1O	13.212999999999999	15.93

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CN1C(=O)O[C@H](C1=O)C2CCCCC21

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN1C(=O)O[C@H](C1=O)C2CCCCC21.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CN1C(=O)O[C@H](C1=O)C2CCCCC21.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CN1C(=O)O[C@H](C1=O)c2ccccc2	12.978999999999999	20.039000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CC(C)(C)[C@H](O)C(=O) C(C)(C)C1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(C)(C)[C@H](O)C(=O)C(C)(C)C1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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Table 1. Results of CDock

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1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CC(C)(C)[C@H](O)C(=O)C(C)(C)C	12.548	18.145

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C[C@@H]1CC(C)(C)N(CCO)C2CC(C)CCC121

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CCNC(=S)SCCC(=O)O	11.699	12.781000000000001

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by CC1=NCCC2C1[NH] C3CC(O)CCC231

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6W4B enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC1=NCCC2C1[NH]C3CC(O)CCC231 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Heptadecane of Bhringaraj plant. The important enzyme of corona virus chosen was 6W4B.

RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1=NCCC2C1[NH]C3CC(O)CCC231.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value CC1=NCCC2C1[NH]C3CC(O)CCC231.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	CC1=NCCc2c1[nH]c3cc(O)ccc23	11.7323	23.155

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by NC1CC(CCC(=O)O) CCC1O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC1CC(CCC(=O)O)CCC1O1.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value NC1CC(CCC(=O)O)CCC1O1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	Nc1cc(CCC(=O)O)ccc1O	25.8897	23.212

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by OC1CC2CCN=CC2CC1O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CC2CCN=CC2CC1O1.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value OC1CC2CCN=CC2CC1O1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	Oc1cc2CCN=Cc2cc1O	12.9391	16.874

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by NN1C=CC2CCCCC2C1 =N1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6W4B enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was NN1C=CC2CCCCC2C1=N1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NN1C=CC2CCCCC2C1=N1.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value NN1C=CC2CCCCC2C1=N1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	NN1C=Cc2ccccc2C1=N	14.0847	16.7985

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by CC(C)COC1=CC(=O) CCC11

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6W4B enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(C)COC1=CC(=O)CCC11 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)COC1=CC(=O)CCC11.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value CC(C)COC1=CC(=O)CCC11.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	CC(C)COC1=CC(=O)CCC1	1.21282	18.1888

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by CCOC1CCC(\C=C\C)CC1O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	CCOc1ccc(\C=C\C)cc1O	4.11943	15.8966

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by CC(C)C1CC(SC#N)C(C)CC1O1

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Table 1. Results of CDock

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1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	CC(C)c1cc(SC#N)c(C)cc1O	9.70993	13.832

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by CCC1=C(C(=O)OC)C(=O)[C@H](C)O11

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

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CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	CCC1=C(C(=O)OC)C(=O)[C@H](C)O1	1.17559	22.4979

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by CNC(=O)OC1CCCC2CCCCC121

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CNC(=O)OC1CCCC2CCCCC121.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value CNC(=O)OC1CCCC2CCCCC121.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	CNC(=O)Oc1cccc2ccccc12	11.5178	22.4121

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by OC1CCCCC1C(=C)N2 CCNC21

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The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value OC1CCCCC1C(=C)N2CCNC21.

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2	Pharmacophore	Oc1ccccc1C(=C)n2ccnc2	12.0738	21.9081

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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2	Pharmacophore	NC1=NN(CC1)c2ccccc2	4.73274	4.73274

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RESEARCH ARTICLE

Deactivation Deactivation of 6W4B Enzyme of Corona by CN1CNC(C(=O)O)C1C (=O)O1

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2	Pharmacophore	Cn1cnc(C(=O)O)c1C(=O)O	18.2363	23.1072

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by C[NH2+]CC(=O)C1CCC(O)C(O)C11

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2	Pharmacophore	C[NH2+]CC(=O)c1ccc(O)c(O)c1	1.67687	6.49116

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RESEARCH ARTICLE

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"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Heptadecane of Bhringaraj plant. The important enzyme of corona virus chosen was 6W4B.

RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC(=S)NC1CCCCC1O1.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value NC(=S)NC1CCCCC1O1.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Heptadecane	36.4839	37.6824
2	Pharmacophore	NC(=S)Nc1ccccc1O	12.7359	17.1563

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by OC1CC([O-])NC2CCCC C121

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6W4B enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was OC1CC([O-])NC2CCCCC121 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1CC([O-])NC2CCCCC121.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value OC1CC([O-])NC2CCCCC121.

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2	Pharmacophore	Oc1cc([O-])nc2ccccc12	12.2063	22.3502

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RESEARCH ARTICLE

Deactivation of 6W4B Enzyme of Corona by OC(=O)C[NH2+]CC1 CCCCC11

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RESULTS AND DISCUSSION

Table 1 shows that Heptadecane can block 6W4B enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC(=O)C[NH2+]CC1CCCCC11.

CONCLUSIONS

The results suggested that Heptadecane can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6W4B enzyme had SMILES value OC(=O)C[NH2+]CC1CCCCC11.

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2	Pharmacophore	OC(=O)C[NH2+]Cc1ccccc1	12.9571	15.5016

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by COC1CC(CN2CNNN2)CCC1O1

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Received: 24 Mar 2020 Revised: 25 Apr 2020 Accepted: 26 May 2020

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC1CC(CN2CNNN2)CCC1O1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value COC1CC(CN2CNNN2)CCC1O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	COc1cc(Cn2cnnn2)ccc1O	2.2829999999999999	17.143000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C[NH+]1CCN (CC2CCCCC2)CC11

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value C[NH+]1CCN(CC2CCCCC2)CC11.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value C[NH+]1CCN(Cc2ccccc2)CC1.

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2	Pharmacophore	C[NH+]1CCN(Cc2ccccc2)CC1	2.1499999999999999	13.220000000000001

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RESEARCH ARTICLE

Deactivation Deactivation of 6M3M Enzyme of Corona by O=C1CC[C@H](O1) C2CCC3CCCCC3C21

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value O=C1CC[C@H](O1)C2CCC3CCCCC3C21.

CONCLUSIONS

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SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
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2	Pharmacophore	O=C1CC[C@H](O1)c2ccc3ccccc3c2	2.073	18.797000000000001

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RESEARCH ARTICLE

Deactivation Deactivation of 6M3M Enzyme of Corona by OC1=C(CC2CCCCC2)C(=O) C3C(O)CCC4CCCC1C341

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Keywords: Corona, Virus, Docking, Biovia

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Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC1=C(CC2CCCCC2)C(=O)C3C(O)CCC4CCCC1C341.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC1=C(Cc2ccccc2)C(=O)c3c(O)ccc4cccc1c34.

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2	Pharmacophore	OC1=C(Cc2ccccc2)C(=O)c3c(O)ccc4cccc1c34	1.919	29.312000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by O[C@@H]1CNC2C(C1)CCC3CCCCC231

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CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CNC(=O)Oc1cccc2ccccc12.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CNC(=O)Oc1cccc2ccccc12	1.5760000000000001	14.944000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by OC(=O)CSCC1CCCC2CCCCC121

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was OC(=O)CSCC1CCCC2CCCCC121 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value OC(=O)CSCC1CCCC2CCCCC121.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value OC(=O)CSCc1cccc2ccccc12.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	OC(=O)CSCc1cccc2ccccc12	1.452	16.347000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CN(C)C(=O)N1CCN(CC1)C(=O)N(C)C1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN(C)C(=O)N1CCN(CC1)C(=O)N(C)C1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CN(C)C(=O)N1CCN(CC1)C(=O)N(C)C.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	CN(C)C(=O)N1CCN(CC1)C(=O)N(C)C	1.395	22.709

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by CLC1NCN(C2=CC(=O)CCC2)C1CL1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CLC1NCN(C2=CC(=O)CCC2)C1CL1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CLC1NCN(C2=CC(=O)CCC2)C1CL1.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value CLC1NCN(C2=CC(=O)CCC2)C1CL.

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2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	Clc1ncn(C2=CC(=O)CCC2)c1Cl	1.1399999999999999	17.175000000000001

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RESEARCH ARTICLE

Deactivation of 6M3M Enzyme of Corona by C1CN(CCO1)SSN2C COCC21

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M3M enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was C1CN(CCO1)SSN2CCOCC21 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5].The pharmacophore that was identified had similarity in structure with Curcumin of Turmeric plant. The important enzyme of corona virus chosen was 6M3M.

RESULTS AND DISCUSSION

Table 1 shows that Curcumin can block 6M3M enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value C1CN(CCO1)SSN2CCOCC21.

CONCLUSIONS

The results suggested that Curcumin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M3M enzyme had SMILES value C1CN(CCO1)SSN2CCOCC2.

REFERENCES

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2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
3. D. Das, S. Das, M. Pandey, D. Bhattacharyay. "In silico Analysis of Phytochemicals from Mucuna pruriens (L.) DC against Mycobacterium tuberculosis Causing Tuberculosis", European Journal of Medicinal Plants (2020) 31(4), 19-24.

Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Curcumin	11.1966	13.2172
2	Pharmacophore	C1CN(CCO1)SSN2CCOCC2	1.0860000000000001	20.786000000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CCOC(CN(C(C)C)C(C)C)OCC1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CCOC(CN(C(C)C)C(C)C)OCC1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CCOC(CN(C(C)C)C(C)C)OCC1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CCOC(CN(C(C)C)C(C)C)OCC.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CCOC(CN(C(C)C)C(C)C)OCC	9.6649100000000008	19.2988

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CN(C)CCS[C@H](CO) C1CCCCC11

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CN(C)CCS[C@H](CO)C1CCCCC11 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN(C)CCS[C@H](CO)C1CCCCC11.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CN(C)CCS[C@H](CO)C1CCCCC1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CN(C)CCS[C@H](CO)c1ccccc1	2.3749500000000001	16.950299999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by NC1=CC(=O)NC(=O) N1CC=C1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

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CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	NC1=CC(=O)NC(=O)N1CC=C	7.8355800000000002	13.7918

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC1(C)OC(=O)C[C@H]1C(=O)O1

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CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC1(C)OC(=O)C[C@H]1C(=O)O	13.172000000000001	15.2887

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(C)COC(=O)OCC(C)C1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(C)COC(=O)OCC(C)C1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)COC(=O)OCC(C)C1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CC(C)COC(=O)OCC(C)C.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(C)COC(=O)OCC(C)C	6.55741	7.4478900000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC1=NN[C@H](C1)C2CCC(O)CC21

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1=NN[C@H](C1)C2CCC(O)CC21.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CC1=NN[C@H](C1)C2CCC(O)CC2.

REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC1=NN[C@H](C1)c2ccc(O)cc2	1.58504	12.274800000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(C)(C)[C@H](O)C(=O) C(C)(C)C1

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ABSTRACT

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Keywords: Corona, Virus, Docking,Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)(C)[C@H](O)C(=O)C(C)(C)C1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CC(C)(C)[C@H](O)C(=O)C(C)(C)C.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(C)(C)[C@H](O)C(=O)C(C)(C)C	10.407400000000001	15.667899999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by COC(=O)[C@](C)(N) CC1CCC(O)CC11

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was COC(=O)[C@](C)(N)CC1CCC(O)CC11 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [5]. The pharmacophore that was identified had similarity in structure with Quercetin of Champa plant. The important enzyme of corona virus chosen was 6M03.

RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COC(=O)[C@](C)(N)CC1CCC(O)CC11.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value COC(=O)[C@](C)(N)CC1CCC(O)CC1.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	COC(=O)[C@](C)(N)Cc1ccc(O)cc1	18.756399999999999	17.009499999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(=O)OC(OC(=O)C)C(=C)C1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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2	Pharmacophore	CC(=O)OC(OC(=O)C)C(=C)C	9.1529500000000006	17.259599999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC1(C)CC(O)CC(C)(C)N1O1

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Keywords: Corona, Virus, Docking, Biovia

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Table 1. Results of CDock

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC1(C)CC(O)CC(C)(C)N1O	3.3019599999999998	17.6676

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RESEARCH ARTICLE

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Keywords: Corona, Virus, Docking, Biovia

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CONCLUSIONS

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CCOC(=O)[C@](C)(OC(=O)C)C(=O)C	24.626200000000001	23.225999999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(C)C1=CC(=O)OC2 C3CCCN4CCCC(CC12)C341

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(C)C1=CC(=O)OC2C3CCCN4CCCC(CC12)C341.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CC(C)C1=CC(=O)OC2C3CCCN4CCCC(CC12)C34.

REFERENCES

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(C)C1=CC(=O)Oc2c3CCCN4CCCc(cc12)c34	5.2497600000000002	17.7346

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(=O)OC1CCC2CCC[N+](C)C2C11

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6M03 enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CC(=O)OC1CCC2CCC[N+](C)C2C11 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)OC1CCC2CCC[N+](C)C2C11.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CC(=O)OC1CCC2CCC[N+](C)C2C1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(=O)Oc1ccc2ccc[n+](C)c2c1	4.5164900000000001	19.939299999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by NC1CCC2CCCC(O)C2N11

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC1CCC2CCCC(O)C2N11.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value NC1CCC2CCCC(O)C2N1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	Nc1ccc2cccc(O)c2n1	4.5528399999999998	11.658300000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC(=C1C(=O)CC(C)(CC1=O)C(=O)O)O1

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=C1C(=O)CC(C)(CC1=O)C(=O)O)O1.

CONCLUSIONS

The results suggested that Quercetin can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6M03 enzyme had SMILES value CC(=C1C(=O)CC(C)(CC1=O)C(=O)O)O.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC(=C1C(=O)CC(C)(CC1=O)C(=O)O)O	3.5807799999999999	19.804300000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC1=CC(=O)O[C@@H](O1)C(C)(C)C1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Quercetin can block 6M03 enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1=CC(=O)O[C@@H](O1)C(C)(C)C1.

CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	CC1=CC(=O)O[C@@H](O1)C(C)(C)C	5.27928	14.191800000000001

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC1(C)CC(CC(C)(C)N1O)C(=O)O1

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	CC1(C)CC(CC(C)(C)N1O)C(=O)O	2.3862100000000002	14.725099999999999

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CC1CCC(CC1)S(=O) (=O)[N-]CL1

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Keywords: Corona, Virus, Docking, Biovia

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1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	Cc1ccc(cc1)S(=O)(=O)[N-]Cl	8.92136	14.3566

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by CCOC(OCC)N1CCNC11

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RESEARCH ARTICLE

Deactivation of 6M03 Enzyme of Corona by COC1CC(CC(OC)C1O)C(=O)C1

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	quercetin	11.1966	13.2172
2	Pharmacophore	COc1cc(cc(OC)c1O)C(=O)C	11.2567	18.2989

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC(=O)C1CC2CCCCC2C(O)C1O

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ABSTRACT

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RESULTS AND DISCUSSION

Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)C1CC2CCCCC2C(O)C1O.

CONCLUSIONS

The results suggested that Gallic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6LVN enzyme had SMILES value CC(=O)c1cc2CCCCc2c(O)c1O.

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2	Pharmacophore	CC(=O)c1cc2CCCCc2c(O)c1O	6.50099	7.54261

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by C[C@H]1C[C@H](CC(C)(C)C1)OC=O

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ABSTRACT

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	C[C@H]1C[C@H](CC(C)(C)C1)OC=O	1.19201	9.58498

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC1(C)N(O)[C@H](NC1=S)C2CCCCC2

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Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	CC1(C)N(O)[C@H](NC1=S)c2ccccc2	2.34666	10.3105

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by NNC(=O)C(=O)NC1 CCCCC1

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	NNC(=O)C(=O)NC1CCCCC1	3.99068	11.1248

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CCOC(=O)CNC(C)(C)C

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by COC(=O)CS[C@H](C)CC(=O)OC

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2	Pharmacophore	COC(=O)CS[C@H](C)CC(=O)OC	15.6469	16.2845

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RESEARCH ARTICLE

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RESEARCH ARTICLE

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	Cc1ccc(O)c(c1)C(=O)NO	10.7078	14.6491

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CN1C(=O) N=C(N)N=C1C (C)(C)C

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6LVN enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was CN1C(=O)N=C(N)N=C1C(C)(C)C (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN1C(=O)N=C(N)N=C1C(C)(C)C.

CONCLUSIONS

The results suggested that Gallic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6LVN enzyme had SMILES value CN1C(=O)N=C(N)N=C1C(C)(C)C.

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2	Pharmacophore	CN1C(=O)N=C(N)N=C1C(C)(C)C	1.64402	13.0573

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC1CC(C)C(CC(=O)O)C(C)C1

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Keywords: Corona, Virus, Docking, Biovia

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Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC1CC(C)C(CC(=O)O)C(C)C1.

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The results suggested that Gallic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6LVN enzyme had SMILES value CC1CC(C)C(CC(=O)O)C(C)C1.

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2	Pharmacophore	Cc1cc(C)c(CC(=O)O)c(C)c1	14.6588	13.6477

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CNC(=O)OC1CCCC2CCCCC12

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CNC(=O)OC1CCCC2CCCCC12.

CONCLUSIONS

The results suggested that Gallic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6LVN enzyme had SMILES value CNC(=O)OC1CCCC2CCCCC12.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	CNC(=O)Oc1cccc2ccccc12	1.61211	15.0121

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CN1C(=O)O[C@H](C1=O)C2CCCCC2

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Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

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RESULTS AND DISCUSSION

Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN1C(=O)O[C@H](C1=O)C2CCCCC2.

CONCLUSIONS

The results suggested that Gallic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6LVN enzyme had SMILES value CN1C(=O)O[C@H](C1=O)C2CCCCC2.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	CN1C(=O)O[C@H](C1=O)c2ccccc2	4.20096	11.4814

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CN1CNC(C(=O)O)C1C (=O)O

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

The pharmacophore that was identified had similarity in structure with Gallic acid of Champa plant. The important enzyme of corona virus chosen was 6LVN. Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CN1CNC(C(=O)O)C1C(=O)O.

CONCLUSIONS

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	Cn1cnc(C(=O)O)c1C(=O)O	5.68902	8.14259

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CCOC(=O)[C@@H]1C [NH2+] CCC1=O

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Keywords: Corona, Virus, Docking, Biovia

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by C[NH2+]CC(=O) C1CCC(O) C(O)C1

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by [O-]C(=O)C(=O)CC1 CCCCC1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6LVN enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was [O-]C(=O)C(=O)CC1CCCCC1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

INTRODUCTION

"Corona virus disease 2019 (COVID-19)" has shaken the whole world by killing many people. [1] A new species of corona named as "COVID-19" caused this attack. The issue is that there is no drug discovered. [2] The mankind is doing research to develop new medicines. The objective of the present work is to identify a medicine against corona.

METHODOLOGY

"Biovia Discovery studio CDOCK and Pharmacophore" menu ("Dassault Systemes, France") were utilized. Pharmacophore menu was used to identify a molecule similar to a ligand. Then CDOCK operation was done between an enzyme of the virus and the ligand. The CDOCK menu used Charmm protocol for docking and gave the "-CDOCK Energy and -CDOCK interaction energy". A positive value indicated blocking of active site of viral enzyme [3].The pharmacophore that was identified had similarity in structure with Gallic acid of Champa plant. The important enzyme of corona virus chosen was 6LVN.

RESULTS AND DISCUSSION

Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value [O-]C(=O)C(=O)CC1CCCCC1.

CONCLUSIONS

The results suggested that Gallic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6LVN enzyme had SMILES value [O-]C(=O)C(=O)CC1CCCCC1.

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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	[O-]C(=O)C(=O)Cc1ccccc1	8.91938	15.6178

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by C[C@@H]([C@H](O)c1ccccc1) [NH+](C)C

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Keywords: Corona, Virus, Docking, Biovia

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Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value C[C@@H]([C@H](O)c1ccccc1)[NH+](C)C.

CONCLUSIONS

The results suggested that Gallic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6LVN enzyme had SMILES value C[C@@H]([C@H](O)c1ccccc1)[NH+](C)C.

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2	Pharmacophore	C[C@@H]([C@H](O)c1ccccc1)[NH+](C)C	2.27602	11.9259

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by NC(=S)Nc1ccccc1O

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value NC(=S)Nc1ccccc1O.

CONCLUSIONS

The results suggested that Gallic acid can fight against corona virus. "Discovery Studio pharmacophore and Cdock module of Biovia software" suggested that the compound capable of deactivating 6LVN enzyme had SMILES value NC(=S)Nc1ccccc1O.

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2	Pharmacophore	NC(=S)Nc1ccccc1O	6.76447	10.8148

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by COc1cc(Cl)ccc1O

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Keywords: Corona, Virus, Docking, Biovia

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RESULTS AND DISCUSSION

Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value COc1cc(Cl)ccc1O.

CONCLUSIONS

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by COC(=O)[C@@H]1[C@H](C)CC(=CC1=O)O

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by OC(=O)C[NH2+]CC1 CCCCC1

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2	Pharmacophore	COC(=O)[C@H](CC(=O)O)C(C)C	19.6093	16.1839

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RESULTS AND DISCUSSION

Table 1 shows that Gallic acid can block 6LVN enzyme of corona virus. A compound was found to be capable of curing the disease by blocking the enzyme had SMILES value CC(=O)NC1CCC(CC1)S(=O) (=O)NC2 (CCCCC2)C(=O)O.

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REFERENCES

1. Statement on the second meeting of the International Health Regulations (2005) Emergency Committee regarding the outbreak of novel coronavirus (2019-nCoV)". World Health Organization (WHO). (2020).
2. H. Iqbal, U. Ria, U. Rooh, K. Muhammad, U. Naseem, A. Basee, K. Farhat, K. Muhammad, Z. Muhammad, J. Khan, N. Khan. Phytochemical analysis of selected medicinal plant. African Journal of Biotechnology. (2011)10, pp. 7487-7492.
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Table 1. Results of CDock

SL NO	Type	Compound	"- C DOCKER ENERGY"	"- C DOCKER INTERACTION ENERGY"
1	Phytochemical	Gallic acid	21.9761	18.3891
2	Pharmacophore	CC(=O)Nc1ccc(cc1)S(=O)(=O)NC2(CCCCC2)C(=O)O	7.17935	13.6327

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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by NC1CCC2CC3CCC(N) CC3S(=O)(=O)C2C1

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ABSTRACT

"Coronavirus disease 2019 (COVID-19)" causes "severe acute respiratory syndrome". Pharmacophore analysis followed by molecular docking utilizing "Biovia Discovery studio" were done and the chemical that can deactivate 6LVN enzyme of corona virus was identified. Based on positive values of "-CDocker energy as well as -CDocker interaction energy" the drug identified was NC1CCC2CC3CCC(N) CC3S(=O)(=O)C2C1 (SMILES).

Keywords: Corona, Virus, Docking, Biovia

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2	Pharmacophore	Nc1ccc2Cc3ccc(N)cc3S(=O)(=O)c2c1	3.441	11.1739

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RESEARCH ARTICLE

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1	Phytochemical	Gallic acid	21.9761	18.3891
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RESEARCH ARTICLE

Deactivation of 6LVN Enzyme of Corona by CC(=O)NC(NC(=O)C) C(=O)C1CCCCC1

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2	Pharmacophore	CC(=O)NC(NC(=O)C)C(=O)c1ccccc1	15.6596	17.4343

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RESEARCH ARTICLE

Design and Development of Automatic Smart Control System for Water Sprinkling and Ventilation

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ABSTRACT

The present invention proposes an automatic control system for water sprinkling and ventilation. The system comprises a circuit board that mechanically supports and electrically connects the components using conductive tracks and there of. The system uses an arduino based ATmega microcontroller that is specifically programmed to compute the input signals. The signals are received from the various sensors that sense moisture content of beds, humidity and ambient temperature and thereof. This is achieved by using a detecting unit with plurality of detectors arrangement for an effective system. Once the controller receives this signal, it begins the process of computation in order to carry out the necessary action for comparing the precise parameters that are pre fed and displayed in a visual means, which makes it very much informative. The system reduces human intervention and takes care of proper maintenance of growth parameters and minimizing wastage of resources in the mushroom cultivation chamber.

Keywords: system, parameters, humidity, temperature, signals, sensors.

INTRODUCTION

The present invention relates to a mushroom cultivation equipment and in particularan environmental condition that can be adjusted to control a mushroom house automationand control systems.

Background of the invention

Diversification in any farming system imparts sustainability. Mushrooms are onesuch component that imparts diversification. One of the major areas that can configuretowards the goal of conservation of natural resources as well as increased productivity isrecycling of agro-wastes including agro-industrial waste. Utilizing these wastes for growingmushrooms can enhance income and impart higher level of sustainability. Large quantities of mushroom production is generally in the greenhouse cultivation,since there are stringent requirements, like very less sun light, temperature and humidity asbeyond a certain range will shadow their growth, thus affecting the production ofmushrooms, the taste and the like. The current control method cannot be practised byartificially resorted temperature and humidity conditions. The production is not maintainedin a relatively stable range if the weather affect is relatively high, so stability of themushroom growing is poor and it is not easy to control the temperature, humidity and otherfactors which effect the production of mushroom growing.

For mushroom cultivation, the environment must be oxygen-free. Existence ofpeople in the salon may cause pollution of the compost and the environment changes thetemperature. On the other hand, working in an oxygen-free environment can harm workers. However, the current control cannot be done by artificially resorted temperature andhumidity conditions; that are affected by the weather which is relatively large, less stable,not easy to control and the like factors. Existence of people in the salon may cause pollutionof the compost and environment and thus change the temperature. Working in an oxygen-free environment can harm workers. Hence, there is a necessity to provide artificiallyresorted temperature and humidity conditions and should be maintained in a relativelystable range. There is a necessity to provide easy operation to control the variablecharacteristics such as moisture, soil type, humidity, carbon dioxide (CO2), temperature,electric conductivity and thereof. There is a necessity to provide automatic operation of thevariable apparatus such as sprinklers, ventilators and thereof at the mushroom cultivationchamber.

Objectives of the invention

1. The primary objective of the invention is to provide automatic sprinkler system forthe mushroom cultivation chamber.
2. The other objective of the invention is to provide automatic air ventilation systemfor the mushroom cultivation chamber.
3. The other objective of the invention is to provide disinfection to the cultivationchamber.
4. The other objective of the invention is to provide stable maintenance of the soilmoisture, humidity and temperature.
5. Further objective of the invention is to provide control unit to control the apparatusas required for attaining certain parameters.

Summary of the Invention

The invention proposes an automatic control system for water sprinkling andventilation. The following presents a simplified summary in order to provide a basicunderstanding of some aspects of the claimed subject matter. This summary is not anextensive overview. It is not intended to identify key/critical elements or to delineate thescope of the claimed subject matter. Its' sole purpose is to present some concepts in asimplified form as a prelude to the more detailed description that is presented later. The automatic control system for water sprinkling and ventilation comprises acontroller to control the apparatus as required to attain the parameters. The controller maybe a microcontroller of Arduino Uno, 8051, ATmega328, AVR, PIC and the like controllers.The controller controls the operation of the variable apparatus by means array of relays.The variable apparatus may be a spray device, a ventilation system, pressurized boosterpump and the like. A detecting unit is provided to detect variable characteristics such asmoisture, soil type, humidity, carbon dioxide (CO2), temperature, electric conductivity andthe like of the mushroom cultivation chamber. The detecting unit includes soil moisturedetector, humidity detector, temperature detector/meter and carbon dioxide (CO2) detector and there of. According to an aspect of the invention,

the system further comprises a spray deviceto maintain the humidity level. The spray devices may be humidifying sprinklers, foggers,water jets, nozzles and thereof to maintain humidity level at the mushroom cultivationchamber. A ventilation system is provided to the cultivation chamber for proper ventilation.The ventilation system is for continuous air supplying means and withdrawing means forcontinuous air supplying by means of fans, blowers and thereof which are to communicatewith ventilation ducts in the said chamber. According to an aspect of the invention, the system further comprises a display todemonstrate real-time data of variable characteristics. The display unit may be a liquidcrystal display (LCD), a light-emitting diode (LED), a vacuum fluorescent display and the like.

Description of Drawings

The accompanying drawings, which are incorporated in and constitute a part of thespecification, illustrate an embodiment of the invention, and, together with the description,serve to explain the principles of the invention.

Detailed description of Drawings

An exemplary embodiment of the present invention will be described in reference tothe accompanying drawings. Wherever possible, same or similar reference numerals areused in the drawings and the description to refer to the same or like parts or steps. FIG. 1 illustrates an automatic sprinkler and ventilation 100 for mushroom cultivationaccording to an embodiment of the invention. The automatic sprinkler and ventilationsystem 101 for mechanically supporting and electrically connecting the electroniccomponents using conductive tracks, pads and other features etched from copper sheetslaminated onto a non-conductive substrate. The system 101 comprises a transformer (3A,12V), 102 may be a step down transformer, an AC-DC adapter 103 for different outputvoltages, a controller 104 to control apparatus, a relay board 105, a water pump 106, an airventilation system 107, a detecting unit 108 and a visual means 109 for demonstrating real-time data of variable characteristics. According to an embodiment of the invention, the AC power supply for providingpower to thesystem, where the transformer 102 steps down the power to 3A and 12V. Theoutput of the transformer 102 i.e., step down power (3A, 12V) is for supplying to the AC toDC adapter 103 for different output voltages i.e., 5V, 9V and 12V and thereof.

The output of the AC to DC adapter 103 i.e., 5V supply is connected to the controller104 and 12V supply is connected to the relay board 105 by means of a cable or any otherlike means. The controller 104 may be a microcontroller of Arduino Uno, 8051, ATmega328,AVR, PIC and the like controllers. For an exemplary embodiment, the system uses ArduinoUno board based on the ATmega328. Most Arduino boards consist of an Atmel 8-bit AVRmicrocontroller (ATmega8, ATmega168, ATmega328, ATmega1280, ATmega2560) withvarying amounts of flash memory, pins, and features. It has 14 digital input/output pins (ofwhich, 6 can be used as PWM outputs), 6 analog inputs, a 16 MHz crystal oscillator, a USBconnection, a power jack, an ICSP header, and a reset button. It is simply connected to acomputer with a USB cable or power supply with an AC/DC adapter or a battery to start.

The output of the AC to DC adapter 103 i.e., 12V supply is connected to the relayboard 105. Relays are used to control the circuit by a low-power signal with completeelectrical isolation between the control and the controlled circuits or where several circuitsmust be controlled by one signal. The pressurized water pump 106and air ventilation 107 isconnected through the relay board 105. The relay board 105 operates the pressurized waterpump 106 and air ventilation 107 based on the variable characteristics such as moisture,humidity, temperature and the like detected by the system. According to an embodiment of the invention, the detecting unit 108 is connected tothe controller 104. The detecting unit 108 includes soil moisture detector, humidity andtemperature detector (DHT11) and carbon dioxide (CO2) detector and thereof. Thecontroller 104 controls the apparatus as it is required to attain variable characteristics suchas moisture, humidity, temperature and the like at the mushroom cultivation chamber.

The soil moisture sensor measures the volumetric water content indirectly by usingsome other properties of the soil, such as electrical resistance, dielectric constant orinteraction with neutrons, as a proxy for the moisture content. The humidity andtemperature detector i.e., DHT11 is a basic, ultra low-cost digital temperature and humiditysensor. It

uses a capacitive humidity sensor and a thermistor to measure the surroundingair, and spits out a digital signal on the data pin (no analog input pins needed). It is fairlysimple to use, but requires careful timing to grab the data. The system further comprises a visual means 109 to demonstrate real-time data ofvariable characteristics. The visual means 109 may be a liquid-crystal display (LCD), a light-emitting diode (LED), a vacuum fluorescent display and the like. For an exemplaryembodiment of the invention, the system uses a flat liquid-crystal display (LCD), a paneldisplay electronic visual display or video display that uses the light modulating properties ofthe liquid crystals. The system uses a monochromatic 20 X 4 alphanumeric LCD. 20 X 4means that 20 characters can be displayed in each of the 4 rows of the 20 X 4 LCD, thus atotal of 80 characters can be displayed at any instance of time.

Fig. 2 illustrates a soil moisture detector 200 according to an embodiment of theinvention. The soil moisture sensor measures the volumetric water content indirectly byusing some other properties of the soil, such as electrical resistance, dielectric constant orinteraction with neutrons, as a proxy for the moisture content. The relation between themeasured property and soil moisture must be calibrated and may vary depending onenvironmental factors such as soil moisture, temperature, or electric conductivity. Reflectedmicrowave radiation is affected by the soil moisture and is used for remote sensing inhydrology and agriculture. By plugging the power cord in the board 101 is to supply 230V AC. The circuit board101 automatically converts into the required DC voltage by means of AC to DC adapter103.The detecting unit with several detectors are connected to the controller 104 and thereby activated. The detecting unit detects the variable characteristics such as moisture,humidity, temperature and carbon dioxide (CO2) and the like of the mushroom cultivationchamber.

The collected values are compared with the programmed values and activate thespray devices accordingly. The pressurized water pump 106 and air ventilation 107 areconnected through a relay board 105 in the circuit board 101 and gets activated based onthe input of the detecting unit, after the comparison of the variable characteristicsaccording to the requirement. After satisfying the variable characteristics of the detectedvalues to that of the predetermined values, the spray devices and air ventilation system ofthe mushroom cultivation chamber may be turned off. The spray devices may be sprinklers, foggers, water jets, nozzles and thereof tomaintain humidity level at the mushroom cultivation chamber. The ventilation system isprovided in the cultivation chamber for continual withdrawal and supply of air by means offans, blowers and thereof and communicating with ventilation ducts in the said cultivationchamber.

The sprinkler devices and air ventilation are activated or deactivated automaticallybased on the detected variable characteristics by means of detecting unit so that theinterior of the cultivation chamber is maintained at a level of suitable moisture content,humidity and temperature in the mushroom growth. This system can reduce pollution and increase safety. For mushroom cultivation, theenvironment must be oxygen-free. Existence of people in the salon may cause change in thetemperature, pollution of the compost and environment. On the other hand, working in anoxygen-free environment can harm the workers. This system reduces the people's entry andpollution of the compost and provides an accurate cultivation with a high efficiency and highamount of crop.

The system provides artificially resorted temperature and humidity conditions andmaintains in a relatively stable range. The system provides an easy control for variablecharacteristics such as moisture, soil type, humidity, carbon dioxide (CO2), temperature,electric conductivity and thereof. The system provides an automatic operation of thevariable apparatus such as sprinklers, air ventilation and pressurized booster pump andthereof at the mushroom cultivation chamber. The system reduces human intervention andtakes care of proper maintenance of the growth parameters and minimization of wastage ofresources. The cost of this system is low and easy for operations.

It will readily be apparent that numerous modifications and alterations can be madeto the processes described in the foregoing examples without departing from the principlesunderlying the invention, and all such modifications and alterations are intended to beembraced by this application.

Claims

We Claim:

1. Automatic control system for water sprinkling and ventilation comprising of:
   a controller to control variable apparatus as required to attain parameters;
   a detecting unit to detect variable characteristics of mushroom cultivation chamber;
   a spray device to maintain humidity levelof mushroom cultivation chamber;
   a ventilation system to maintain proper ventilation in the mushroom cultivationchamber;
   a pressurized booster pump to supply water to the mushroom cultivation chamber;
   and
   a visual means to demonstrate real-time data of variable characteristics.
2. Automatic control system for water sprinkling and ventilation as claimed in claim 1,wherein said controller may be a microcontroller of Arduino Uno, 8051, ATmega328,AVR, PIC and the like controllers.
3. Automatic control system for water sprinkling and ventilation as claimed in claim 1,wherein said controller controls operation of the spray device, ventilation system,pressurized booster pump and the like based on inputs from the detecting unit.
4. 4.Automatic control system for water sprinkling and ventilation as claimed in claim 1,wherein said controller controls operation of the variable apparatus such as fans,sprinklers, detecting unit and thereof using array of relays.
5. Automatic control system for water sprinkling and ventilation as claimed in claim 1,wherein said detecting unit may comprise a soil moisture detector, a humiditydetector, a temperature detector and a carbon dioxide (CO2) detector andthereof,wherein said variable characteristics may be soil moisture, humidity, carbondioxide (CO2), temperature, electric conductivity and thereof.
6. Automatic control system for water sprinkling and ventilation as claimed in claim 1,wherein said spray device may be humidifying sprinklers, foggers, water jets, nozzlesand thereof to maintain humidity level at mushroom cultivation chamber.
7. Automatic control system for water sprinkling and ventilation as claimed in claim 1,wherein said ventilation system may comprise an air supplying means and an airwithdrawing means for continual withdrawal and supply of air by means of fans,blowers and thereof communicating with ventilation ducts in said chamber.
8. Automatic control system for water sprinkling and ventilation as claimed in claim 1,wherein said visual means may be a liquid crystal display (LCD), a light-emittingdiode (LED), vacuum fluorescent display and the like.

CONCLUSION

To increase efficiency and speed, accuracy and to decrease cost, the recent approaches in developing decision support systems for agriculture, and more generally for environmental problems management, tend to adopt a "systemic" approach. So, we have tried to figure out an optimized way in mushroom cultivation. For this purpose, we have introduced a system which can controls the room temperature, humidity and moisture level, interact with each other and decide automatically. The result of implementation shows this methodology provides a considerable speedup in the control mechanism of mushroom cultivation process. The presented methodology provides an infrastructure to increase the speedup of cultivation control process and can be applied to most of agriculture products. Also, in mushroom cultivation, pollution is an important factor that has more effects in the growth of the mushrooms. With using sensors, reduce people entrance and automatic monitoring, we could decrease pollution and increase the amounts of the crops.

REFERENCES

1. D. Tao Yang and Xiaodong Zhu, —Modernization of agriculture and long-term growth, Journal of Monetary Economics, vol. 60, pp. 367-382, 2013.

2. V.K. Tewari, A. Ashok Kumar, Satya Prakash Kumar, and BrajeshNare, —Farm mechanization status of West Bengal in India, Journal of Agricultural Science, vol. 1, pp. 139-146, 2012.
3. Zhang Qiaoning, Ren Wentao, Cui Hongguang, and Liu Hongyu, —Research of Implementation Effect of China Agricultural Mechanization Promotion Law, Journal of Agricultural Mechanization Research, 2013.
4. H.R. Naji, B.E. Wells, and M. Aborizka, —Hardware agents, in Proceedings of the ISCA 11th International Conference on Intelligent Systems on Emerging Technologies (ICIS-2002), Boston, MA, 2002.
5. H. R. Naji, B. E. Wells, and L. Etzkorn, —Creating an adaptive embedded system by applying multi-agent techniques to reconfigurable hardware, Future Generation Computer Systems, vol. 20, pp. 1055-1081, 2004.
6. L. Klein, —Sensor and Data Fusion Concepts and Applications , SPIE Optical Engineering Press, 1999.
7. Michael Kassler,—Agricultural Automation in the new Millennium, Computers and Electronics in Agriculture vol. 30, pp. 237-240, 2001.
8. S. A. Edrees, A. Rafea, I. Fathy, and M. Yahia, —NEPER: a multiple strategy wheat expert system, Computers and Electronics in Agriculture, vol. 40, pp. 27-43, 2003.
9. Ahlawat OP (2003). Survivability of paddy straw mushroom cultures on storing under different conditions. Indian J Mushroom XXI (1&2): 13-18, 2003.
10. Ahlawat OP, Ahlawat K and Dhar BL . Influence of lignocellulolytic enzymes on substrate colonization and yield in monosporous isolates and parent strains of Volvariellavolvacea. Indian J Microbiol 45(3): 205-210, 2005.
11. Ahlawat OP and Kumar Satish . Traditional and modern cultivation technologies for the paddy straw mushroom (Volvariella spp.). In Frontiers in Mushroom Biotechnology (Rai RD, Upadhyay RC and Sharma SR, Eds.) pp. 157164, National Research Centre for Mushroom, Solan (HP), India, 2005.
12. Ahlawat OP, Pardeep Kumar, Rai RD and Tewari RP . Variations in biochemical properties of different strains of Volvariellavolvacea (Bull Fr.) Sing. under different conditions. Indian J Micobiol 46(1): 31-37, 2006.
13. Sarah Wise, and Andrew T. Crooks, —community resource management: Acequia-based agriculture, Computers, Environment and Urban Systems, vol. 36, pp. 562-572, 2012.
14. RémiLemoya, Charles Raux, and Pablo Jensenb, —Polycentric city and multi-worker households: an agent-based microeconomic model, HAL: hal-00602087, pp. 3-27, 2013.

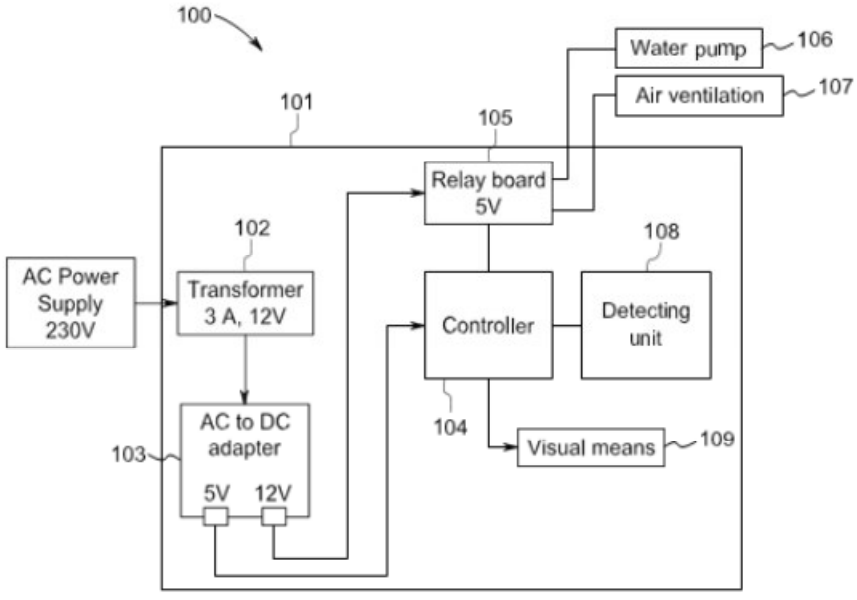

Fig 1. illustrates a block diagram of automatic sprinkler and ventilation system formushroom cultivation according to an embodiment of the invention.

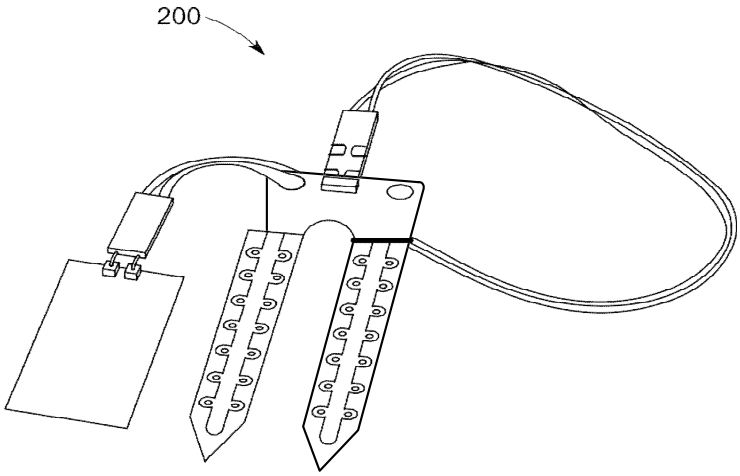

FIG. 2 illustrates a soil moisture sensor according to an embodiment of the invention.

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RESEARCH ARTICLE

Novel Method for Classification of Big Data into Structured Small Data

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ABSTRACT

Big Data is term for datasets that are so large or complex that the traditional data processing application software is inadequate. The use of Big Data has widely spread during the recent times. All the multimillion companies has started implementing methods to make the best use of it. Big Data has its own share of challenges to be dealt with. As the data is really large the retrieving of useful information and classifying the data is a huge challenge.The software experts strived hard in developing the algorithms for classifying and retrieving the data required. The retrieving is dependent on queries produced by the user. In our project we implement a classification algorithm called KNN (K Nearest Neighbors) that classifies the data and gives a map of the nearest neighbors.

Keywords: Big Data, Data sets, Classification, Queries.

INTRODUCTION

Aim: The aim of our project is the software experts strived hard in developing the algorithms for classifying and retrieving the data required. The retrieving is dependent on queries produced by the user. In our project we implement a classification algorithm called KNN (K Nearest Neighbors) that classifies the data and gives a map of the nearest neighbors.

History: Big data is a term for data sets that are so large or complex that traditional data processing application software is inadequate to deal with them. Challenge includes capture, storage, analysis, data curation, and search,

sharing, transfer, visualization, querying, updating and information privacy. The term "Big Data" often refers simply to the use of predictive analysis, user behaviour analytics, or certain other advanced data analytical methods that extract value from data, and seldom to a particular size of the data set. There is little doubt that the quantities of data now available are indeed large, but that's not the most relevant characteristic of this new data ecosystem. Analysis of data sets can find new correlations to "spot business trends, prevent diseases, and combat crime. Scientists, business executives, practitioners of medicines, advertising and governments alike regularly meet difficulties with large data sets in areas including internet search, finance, urban informatics and business informatics.

Description: Data sets grow rapidly – in part because they are increasingly gathered by information-sensing mobile devices, aeriel (remote sensing), software logs, cameras, microphones, Radio Frequency Indentification (RFID) readers and wireless sensor networks. The world's technological per-capita capacity to store information has roughly doubled every 40 months since the 1980s; as of 2012, every day 2.5 extrabytes (2.5×10^{18}) of data are generated. One question for large enterprises is determining who should own big-data initiatives that affect the entire organization. Relational database management systems and desktop statistics- and visualization-packages often have difficulty handling big data. The work may require "massively parallel software running on tens, hundreds, or even thousands of servers". What counts as "big data" varies depending on the capabilities of the users and their tools, and expanding capabilities make big data a moving target. "For some organizations, facing hundreds of gigabytes of data for the first time may trigger a need to reconsider data management options. For others, it may take tens or hundreds of terabytes before data size becomes a significant consideration."

Motivation: The computing revolution that began more than two decades ago has led to large amounts of digital data being amassed by corporations. Advances in digital sensors; proliferation of communication systems, especially mobile platforms and devices; massive scale logging of system events; and rapid movement toward paperless organizations have led to a massive collection of data resources within organizations. And the increasing dependence of businesses on technology ensures that the data will continue to grow at an even faster rate.

Purpose : The concept of Big Data has been around for more than a decade – but while it is potential to transform the effectiveness, efficiency, and profitability of virtually any enterprise has been well documented, the means to effectively leverage Big Data and realize its promised benefits still eludes some organizations. Ultimately, there are two main hurdles to tackle when it comes to realizing these benefits. The first is realizing that the real purpose of leveraging Big Data is to take action – to make more accurate decisions and to do so quickly. We call this situational awareness. Regardless of industry or environment, situational awareness means having an understanding of what you need to know, what you have control of, and conducting analysis in real-time to identify anomalies in normal patterns or behaviors that can affect the outcome of a business or process. If you have these things, making the right decision within the right amount of time in any context becomes much easier.

Scope: A team of statisticians, data scientists and software engineers experienced in handling big data platforms such as Hadoop, MongoDB etc. Inclusion of data from social media and other publicly available sources for better insights and decision making. Integration of Sentiment Analysis engine with Big Data platform to process large volumes of data from internal as well as publicly available sources.

LITERATURE SURVEY

The aim of this section is to provide a review of the research efforts related to effective temperature monitoring systems.

Big Data: The term has been in use since the 1990s, with some giving credit to John Mashey for coining or at least making it popular. Big data usually includes data sets with sizes beyond the ability of commonly used software tools to capture, curate, manage, and process data within a tolerable elapsed time. Big data "size" is a constantly moving target, as of 2012 ranging from a few dozen terabytes to many petabytes of data. Big data requires a set of techniques

and technologies with new forms of integration to reveal insights from datasets that are diverse, complex, and of a massive scale. In a 2001 research report and related lectures, META Group (now Gartner) defined data growth challenges and opportunities as being three-dimensional, i.e. increasing volume (amount of data), velocity (speed of data in and out), and variety (range of data types and sources). Gartner, and now much of the industry, continue to use this "3Vs" model for describing big data. In 2012, Gartner updated its definition as follows: "Big data is high volume, high velocity, and/or high variety information assets that require new forms of processing to enable enhanced decision making, insight discovery and process optimization." Gartner's definition of the 3Vs is still widely used, and in agreement with a consensual definition that states that "Big Data represents the Information assets characterized by such a High Volume, Velocity and Variety to require specific Technology and Analytical Methods for its transformation into Value". Additionally, a new V "Veracity" is added by some organizations to describe it, revisionism challenged by some industry authorities. The 3Vs have been expanded to other complementary characteristics of big data.

Volume: big data doesn't sample; it just observes and tracks what happens **Velocity:** big data is often available in real-time

Variety: big data draws from text, images, audio, video; plus it completes missing pieces through data fusion

Machine learning:big data often doesn't ask why and simply detects patterns

Digital footprint: big data is often a cost-free byproduct of digital interaction. The growing maturity of the concept more starkly delineates the difference between big data and businessintelligence. Business Intelligence uses descriptive statistics with data with high information density to measure things, detect trends, etc. Big data uses inductive statistics and concepts from nonlinear system identification to infer laws (regressions, nonlinear relationships, and causal effects) from large sets of data with low information density to reveal relationships and dependencies, or to perform predictions of outcomes and behaviors.

Advantages:

- **Big Data is Timely** –60% of each workday, knowledge workers spend attempting to find andmanage data.
- **Big Data is Accessible** –Half of senior executives report that accessing the right data is
- difficult.
- **Big Data is Holistic** –Information is currently kept in silos within the organization.Marketing data, for example, might be found in web analytics, mobile analytics, social analytics, CRMs, A/B Testing tools, email marketing systems, and more each with focus on its silo.
- **Big Data is Trustworthy** –29% of companies measure the monetary cost of poor dataquality. Things as simple as monitoring multiple systems for customer contact informationupdates can save millions of dollars.
- **Big Data is Relevant** –43% of companies are dissatisfied with their tools ability to filter outirrelevant data. Something as simple as filtering customers from your web analytics can provide a ton of insight into your acquisition efforts.
- **Big Data is Secure** –The average data security breach costs $214 per customer. The secureinfrastructures being built by big data hosting and technology partners can save the averagecompany 1.6% of annual revenues.
- **Big Data is Authoritative** –80% of organizations struggle with multiple versions of the truthdepending on the source of their data. By combining multiple, vetted sources, more companies can produce highly accurate intelligence sources.
- **Big Data is Actionable** –Outdated or bad data results in 46% of companies making baddecisions that can cost billions.

Applications

- Health Care
- Education
- Media
- Manufacturing
- Internet of Things(IOT)
- Retail

Description: Big Data is a phrase used to mean a massive volume of both structured and unstructured data that is so large that it is difficult to process using traditional database and software techniques. In most enterprise scenarios the volume of data is too large or too fast as it exceeds current processing capacity. Big Data has the potential to help companies improve operations and make faster, more intelligent decisions. This data, when captured, formatted, manipulated, stored and analysed can help a company to gain useful insight to increase revenues, get or retain customers and improve operations. Big data is the term that may seem to reference volume of data. But in case of vendors, it may refer to technology that an organization required to handle the amounts of data and storage. The technology consists of tools and processes.

Volume: Organizations collect data from a variety of sources, including business transactions, social media and information from sensor or machine-to-machine data. In the past, storing it would have been a problem – but new technologies (such as hadoop) have eased the burden.

Velocity: Data streams in at an unprecedented speed and must be dealt with in a timely manner. RFID tags, sensors and smart metering are driving the need to deal with torrents of data in near-real time.

Variety: Data comes in all type of formats from structured, numeric data in traditional databases to unstructured text documents, email, video, audio, stock ticker data and financial transactions.

Variability: In addition to the increasing velocities and varieties of data, data flows can be highly inconsistent with periodic peaks. Is something trending in social media? Daily, seasonal and event-triggered peak data loads can be challenging to manage.

Complexity: Data comes from multiple sources, which makes it difficult to link, match, cleanse and transform data across systems. However, its necessary to connect and correlate relationships, hierarchies and multiple links or your data can quickly spiral out of control.

Potential: As the data keeps growing day by day the need for big data keeps raising. The data on global level is almost inconceivable and it keeps growing. It is estimated that all the information the world has acquired till 2013 is equal to the amount that we got in the next two years. The big data has the potential to store, search and retrieve all this information to us. It is probably the only source in the world right now that can help us the growing data. It can be embedded with the latest technologies like IOT, Neural Networks to get the better results. The data we receive has already been revolutionized during the recent times by developing the means of social networking and it can only get better with big data.

Review on Big Data

In the current scenario, Web and its associated entity, Internet, a shadow has been cast on the same with the data explosion that has taken place in the last couple of years considering the interaction that has been taking place between people and systems associated at multiple touch points. This huge entity which is taking place at every touch point as mentioned above in its wholesome behaviour is known as Big Data. Some decades earlier, Kilobytes and Megabytes used to be entities, which used to combine the entire definition of data existing on the planet, and

due to continuous interactions between people and systems that have been taking place which has lead to exponential growth of data due to which new terms such as Gigabytes, Terabytes, Petabytes,Exabyte's & Zettabytes have graced the steps of the computing world. Theorists and Researchers have propagated this that as Moore's law was to growth of transistors inside the circuits, Data inInternet would exceed the entire brain capacity of the living species. Technological advances have been taking place continuously across all the domains and the major reasons for it are advances in digital sensors, computation, communications and storage that have created humongous collection of data. As explained above, data is generated through various sources which will be used by multiple organizations to run and understand the various business scenarios which help them understand and run their business. All the above data when analysed through various sources and methods of data analysis help organizations in studying customer behaviour, interpreting market trends and taking strategic and financial decisions.

When we speak about Big Data, as we have done above, we often identify it as a jargon, catch phrase which means a exponential volume of unstructured and structured data that contains so many huge datasets which cannot be processed by traditional database management techniques and associated software techniques. With the size of the big data and simply the capacity of the data that it encompasses, it carries in itself the potential that will help companies, in making far better, intelligent and data driven decisions and help in improving operations. For most of the organizational scenarios, it can be easily identified either the data is in excess of the current storage and processing capacity, or the volume of the data is too big or it moves too fast. To give insights using the same data, that we have spoken about earlier, it has to help us in giving insights which would help us in gain competitive advantage, increasing revenues and customer retention and for that we need to capture the data, clean the data, format, manipulate, store and analyze the same.

Data Forms

Structured

When we talk about structured data, we often conclusively identify that, as soon as we placed our current data ware house in the relational database management system, the structure of the relational database management system was enforced on the current data ware house system, which is inclusive to understand the meaning associated with it. So we know, which columns are placed where, whom are they associated with and how the columns are associated in between tables and table spaces. The format of the data can be in text or numerical, but it is common understanding that for every person there is a unique identifier in terms of Age.
The entire data is organized in terms of Entities (Semantic Chunks).
Relations or Classes (Similar entities are grouped together).
Attributes (Same descriptions for entities existing in the Same groups)
Schema (All Entities in the group have a description associated with it.

Semi Structured

As we move on from structured data to semi structured data, there is little to demarcate and often the differentiating lines goes blurry. The data format that we are describing here does not conform to an explicit and fixed schema, however the tags associated with the data, if found associated with organizational structure, then the same data would be easier to analyze and organize. The same concept described here would predate the idea of XML but not HTML. Data is available in many formats, in the current scenario, electronically

- Database Systems
- File Systems e.g., Bibliographic data, Web data
- Data Exchange Formats, e.g. EDI, Scientific data
- Data that is not completely structured, but partially as spoken earlier
- Grouping of Similar Entities and semantically organized
- Entities may not have same attributes in the group

Unstructured

We have already discussed about the Structured and Semi Structured formats. Moving on to the unstructured format, this type would consists of formats that cannot be easily indexed. When we talk about indexing, it is with reference of relational tables and for the purpose of querying or analysis. This would include the file types that are associated with audio, video and image files.

Importance of Big Data

Importance would be defined in terms of how effective this concept has been for organizations, in improving their most important KPI's, also not with the quantity of data the organization has, but with the insights that it has helped to generate. Data is taken from multiple source and integrated across various environments which when analyzed can help us give answers to following:

- Time & Cost reductions.
- Customized & Optimized Market Offerings & New Product Development.
- Strategy Development & Smart Decision Making.

In a Business environment, there are a lot of decisions that are to be taken on the basis of Data & associated analytics and in simple terms, we could define it as Big Data when combined with powered analytics, lot of business related tasks can be accomplished such as:

- Root Cause Analysis can be conducted in real time for associated defects, failures and issues.
- POS based generated coupons based on Consumer Behaviour.
- Risk Portfolio – Quick Calculations/Re-Calculations can be conducted in minutes.
- Conducting Fraud Detection & use of Fraud analytics before hitting organization.

Big Data Characteristics: As mentioned before, big data is a concept and the same can be defined through a model and in our case, it can be defined through 3V model, whose definition was casted by Laney, "high-volume, high-velocity and high-variety information assets that demand cost-effective, innovative forms of information processing for enhanced insight and decision making". Recently in 2012, Gartner processed the definition of Big Data as "Big data is high volume, high velocity, and/or high variety information assets that require new forms of processing to enable enhanced decision making, insight discovery and process optimization".

By definitions, both aforementioned incorporate three main features: Volume, Variety, and Velocity. When the concept is spread across organizations and different business models & big data practitioners, the 3V model can be extended to 4V (V for Value added) or 5V (V for Veracity) could be another factors dependent on the organization, which model they want to adapt. Getting a summary of the same, we can easily state that these models, provide a straightforward and all accepted definitions related to what all is incorporated in a big data based application, solution, problem and framework.

Volume: This would refer to the data from multiple sources, data being in huge capacity. It caninclude all and any kind of data, including the data that is created from all the connected devices, IoT & mobile data and all the data that is being resulted from this communication. In the current scenario, it can be easily stated that, data that is being generated is being approached in computer memory sizes, that were being heard of exabytes, petabytes & zettabytes. It will be coined to reach terms, that are still undefined and new names would have to be though for the same. However, since the data is being generated at the capacity, that we are unable to comprehend, and organizations are still trying to keep up with that pace. Consequences, that are being resulted from these actions, it has become anormalcy for the companies, to store enormous and varied amounts of data : financial, biochemistry, electronics, computer records, genetic, social networks & healthcare. The benefits that are being generated from incorporating

this data, are companies at their disposal have a lot of data, which is a challenges in itself, however, valuable information can be obtained from the same regarding people & companies.

Velocity: When we talk about transferring a movie, than we really do not worry about velocity, forthat movie will be approximately 1 Gigabyte in size and would take a minute to complete. But when we talk about the big data, we can easily state that, for the data that is of the size of exabytes & petabytes, the same data, would take a lot of time to transfer and hence the velocity becomes a very important factor as it affects performance also. When we speak about the data, the contents are constantly changing, via introduction of previous or legacy collections & absorption of complementary data collections and will involve data streamed through multiple sources. Velocity not only involves, the speed at which the data is transferred, but will also involve, data streams, creation of structured records, access to data & delivery. The issues does not only lie with the velocity of incoming data but also to stream outgoing data for batch processing.

Variety: This refers to varied data types and the same can be accumulated from various sources,sources being: social networks, Smartphone, sensors in the forms of videos, images, audio, logs etc. This data can be highly structured (data fetched from the traditional database systems), semi-structured (feeds – social, rss, raw; web logs) or unstructured (clicks, audio, images, videos).

Value: It refers to the critical & valuable information that is being extracted from big datasets thatare associated with the concept of Big Data and this concept in its entirety is called as Big Data Analytics. When we speak about the 4V model, V that stands for Value becomes the most critical factors for any Tanvi, Dr. Radha Krishna Page 26 application based on Big Data & this for the sole reason that it allows to generate useful business information. Till recent times, large volumes of data were recorded as part of regulations but never analysed or exploited. Considering that fact, Value is highly subjective in nature. Big Data as a concept brings with itself the technologies, that enables people & organizations to help exploit the data, the way it was never done before.

Veracity: This term would refer to the accuracy & correctness of the data on which the analysis is tobe conducted. A lot of uncertainties can be caused for the most simple of reasons such as : Data inconsistency, Data Ambiguity, Data Duplications, incompleteness, deception, fraud, duplication, Approximated models, spam & latency. It is not necessary, that the analysis on top of big data, would give a perfect conclusive result. However, everything can be assigned a probability.

Analysis on Big Data

Data Acquisition and Recording: After discussing so much on Big Data, we can safely assume that,Big Data does not simply appear out of thin air. There are multiple sources from which data is recorded. Since we are accumulating so much data, it will be obvious, that part of the data will be of no use & speaking in that way, filtering & compression techniques can be used to sort the matter out. When speaking out about filtering & compressing, we have to take care to define them in such a way, that they should not leave out important information. The other challenge that we would be speaking about is the generation of right metadata to describe the recording of the data and measurement of the same. Also, at the same point of time, we can easily state that, recording the information about the data at the start/birth is not useful since in the pipeline it will keep on changing and interpreted in different ways while being carried through the data analysis stages.

Information Extraction and Cleaning: Simply collecting the information would not help ingenerating analysis or will not be in a state to generate analysis and insights. Data simply in this collected form, will not be in a format which can be analysed. To do this correctly, we need a process which will help us in extracting information, that will help us in pulling out the required information and will be presented in a structured analysis, which will help us in generating insights from the same. Doing the aforementioned process again and again, and that too in a continual manner with correctness being the top priority is a technical challenges that is continuous in nature. Data cleaning is

one of the primary focus areas, that assumes constraints that are well documented and well recognized on valid data or error models that have a deep understanding with reference to the data. For most of the areas, where Big Data emergence is new, these models do not exist.

Data Integration, Aggregation, and Representation: When we speak on the current topic, wewould be talking about Data analysis. Data Analysis is not as simple as the meaning it connotates, for it includes challenges than simple location, identification, understanding & citing data. When we speak about the analysis that is constituted on a large scale, it would be happening in a purely automated fashion. In the current scenario, when we speak about Database Design, it is an art as opposed to science. When we speak about the aforementioned top heroic as science, it has to be developed in a context, whether it being in the Enterprise or Cloud context. Domain Scientists has emerged as a new context, where in they are highly paid professionals along with enabling other professions in the same domain as well, to develop effective database designs. These can be achieved via various ways: design process will be assisted by devising tools, revamping the designing process,development of new techniques and all of them will be used for effective creation of intelligible database design.

Query Processing, Data Modeling, and Analysis: Big data is traditionally different from traditionaldatabase management systems and hence the methods for querying & mining in Big Data are different from traditional statistical techniques which will be different on Big & small samples. When we talk about Big Data, we often associate it with being dynamic, inter-relationships, untrustworthy & noisy as opposed to the process of mining, which will require clean, trustworthy, integrated, efficient, accessible data which can be accessed via mining interfaces using declarative queries, scalable mining algorithms and computing environments for big data. When we are speaking of the aforementioned topics, we can easily state that the data mining itself can be used to help with trust quotient of data as well improving quality of the same, understanding the associated semantics of the data & provide insightful & intelligible querying functions. One of the major problem that Big Data faces is that there is no coordination between the database packages which host the big datasets that are part of the Big Data. Part of the Database systems host the data, part deal with SQL Querying and other ones host the data mining and statistical analysis.

Interpretation: We should understand that analysis is of limited value, if user cannot understand thesame with reference to Big Data. Even if analysis is done all the reports and graphs are generated, one still has to sit and interpret the same. The interpretation cannot happen, while sitting alone in a cubicle or vacuum as the person analysing the reports and graphs has to take care of the assumptions that were used while generating the analysis and retracing the steps.

Big Data Ecosystem: While speaking about the Big Data, we can sense that and would like to statethat, it is a problem, not only related to database or Hadoop, but would constitute technologies at its core and components for data processing on large scale and data analytics. The entire structure of components to analyze by storing, processing, visualizing and delivering results to applications which were the target incorporating Big Data as “fuel” for all the processes which are data related and associated source, target and outcome. All the associations between the components and the intertwined relationships can be incorporated into the BDE or Big Data Ecosystem that will incorporate in itself all the data, supporting infrastructure, models during entire Big Data Lifecycle.

Techniques and Technologies: In the current paper, we will not be giving an in depth overview on the tools and techniques, however, we will be giving an overview of the tools and techniques associated with Big Data. This will help the reader get a association with the tools used for Big Data analytics.

Techniques: There are a lot of techniques that could be used when going to start with a project. Some of the tools which have frequent usage are summarized here.

Association rule learning: A set of techniques for discovering interesting relationships, i.e.,"association rules," among variables in large databases.

Data mining: One of the most important terms related to data-driven decision making and describesit as "searching or 'digging into' a data file for information to understand better a particular phenomenon."

Cluster analysis: Cluster analysis is a type of data mining that divides a large group into smallergroups of similar objects "whose characteristics of similarity are not known in advance."

Crowd sourcing: Crowd sourcing collects data from a large group of people through an open call,usually via a Web2.0 tool. This tool is used more for collecting data than for analyzing it.

Machine learning: Traditionally computers only know what we tell them, but in machine learning, asubspecialty of computer science, we try to craft "algorithms that allow computers to evolve based on empirical data.

Text analytics: A large portion of generated data is in text form. Text Analytics is the process ofconverting unstructured text data into meaningful data.

Technology: As with the analytical techniques, there are several software products and availabletechnologies to facilitate big data analytics. Some of the most common will be discussed here.

EDWs: Enterprise data warehouses are databases used in data analysis.

Visualization products: One of the difficulties with big data analytics is finding ways to visuallyrepresent results. Many new visualization products aim to fill this need, devising methods for representing data points numbering up into the millions. Beyond simple representation visualization can also help in the information search.

MapReduce: MapReduce is a processing technique and a program model for distributed computingbased on java. The MapReduce algorithm contains two important tasks, namely Map and Reduce. Map takes a set of data and converts it into another set of data, where individual elements are broken down into tuples (key/value pairs). Secondly, reduce task, which takes the output from a map as an input and combines those data tuples into a smaller set of tuples.

Hadoop: It is an open-source framework that allows to store and process big data in a distributedenvironment across clusters of computers using simple programming models. Hadoop is an Apache managed software framework derived from MapReduce and Big Table.

NoSQL databases: NoSQL database, also called Not Only SQL, is an approach to data managementand database design that's useful for very large sets of distributed data. NoSQL is especially useful when an enterprise needs to access and analyze massive amounts of unstructured data or data that's stored remotely on multiple virtual servers in the cloud. The most popular NoSQL database is Apache Cassandra. Other NoSQL implementations include SimpleDB, Google BigTable, Apache Hadoop, MapReduce, MemcacheDB, and Voldemort.

Usage Areas of Big Data

Big data is used efficiently in numerous fields. Some of them are listed below:

- Automotive industry
- High technology and industry
- Oil and gas
- Telecommunication sector

- Medical field
- Retail industry
- Packaged consumer products
- Media and show business
- Travel and transport sector
- Financial services
- Social media and online services
- Public services
- Education and research
- Health services
- Law enforcement and defense industry

CONCLUSION

After writing this report/paper, we have developed better understanding of this concept called as Big Data after we have been able to put words to it. We have been able to define models, ecosystems and categorize elements on the basis of it. We also have been able to identify the tools and techniques that have been associated with Big Data Analytics on a frequent basis. On the basis of the analysis conducted, we identified the areas with maximum usage of Big Data Analytics.

SUMMARY

Big Data is the latest technology that stores, searches and retrieves the data for the end user. The tools and software for using this technology are being developed in the recent times by most of the multi-million companies. Our project is an effort that we did in this field using the K-means methods which is an algorithm that is being used in Big Data.

Related work
Requirements
System Requirements

Language	: R
Operating system	: Windows XP, 7, 8
Technologies	: R, RStudio

Hardware Requirements

The following are thebasic hardware requirements that are essential for properexecution of the project.

Processor	: Dual-core with 1.4GHZ or above
RAM Capacity	: >4 GB
Hard Disk	: >50 GB

CSV FILES

A CSV is a comma separated values file which allows data to be saved in a table structured format. CSVs look like a garden-variety spreadsheet but with a **.csv**extension (Traditionally they take the form of a text file containing information separated by commas, hence the name).The term "CSV" also denotes some closely related delimiter-separatedformats that use different field delimiters. These include tab-separated values and space-separated values. A delimiter that is not present in the field data (such as tab) keeps the format parsing simple.

The alternate delimiter-separated files are often even given a .csv extension despite the use of a non-comma field separator. This loose terminology can cause problems in dataexchange. Many applications that accept CSV files have options to select the delimiter character and the quotation character. CSV is a common data exchange format that is widely supported by consumer, business, and scientific applications. Among its most common uses is moving tabular data between programs that natively operate on incompatible (often proprietary and/or undocumented) formats. This works despite lack of adherence to RFC 4180 (or any other standard), because so many programs support variations on the CSV format for data import. For example, a user may need to transfer information from a database program that stores data in a proprietary format, to a spreadsheet that uses a completely different format. The database program most likely can export its data as "CSV"; the exported CSV file can then be imported by the spreadsheet program.

R

R is an open source programming language and software environment for statisticalcomputing and graphics that is supported by the R Foundation for Statistical Computing.[5]The R language is widely used among statisticians and data miners for developing statisticalsoftware and data analysis. R is a GNU package.[9]The source code for the R software environment is written primarily in C, Fortran, and R. R is freely available under the GNUGeneral Public License, and pre-compiled binary versions are provided for various operatingsystems. While R has a command line interface, there are several graphical front-ends available.

HISTORY

R is an implementation of the S programming language combined with lexicalscoping semantics inspired by Scheme.[12]S was created by John Chambers while at Bell Labs. There are some important differences, but much of the code written for S runs unaltered. R was created by Ross Ihaka and Robert Gentleman[14]at the University of Auckland, New Zealand, and is currently developed by the *R Development Core Team*, of which Chambers is a member. R is named partly after the first names of the first two R authors and partly as a play on the name of S. The project was conceived in 1992, with an initial version released in 1995 and a stable beta version in 2000.

HANDLING CSV FILES

In R, we can read data from files stored outside the R environment. We can also write data into files which will be stored and accessed by the operating system. R can read and write into various file formats like csv, excel, xml etc.
Read data from a csv file and then write data into a csv file. The file should be present in current working directory so that R can read it. Of course we can also set our own directory and read files from there.

- Getting and Setting the Working Directory Input a CSV File
- Reading a CSV File
- Analyzing the CSV File

LINE GRAPH

A line chart is a graph that connects a series of points by drawing line segments between them. These points are ordered in one of their coordinate (usually the x-coordinate) value. Line charts are usually used in identifying the trends in data. The **plot()** function in R is used to create the line graph.
The basic syntax to create a line chart in R is −
plot(v,type,col,xlab,ylab)
Following is the description of the parameters used −
v is a vector containing the numeric values.
type takes the value "p" to draw only the points, "l" to draw only the lines and "o" todraw both points and lines.
xlab is the label for x axis.
ylab is the label for y axis.
main is the Title of the chart.

col is used to give colors to both the points and lines. A dataset is taken as an input in the form of CSV file and using the R commands, a line graph is generated which gives a clear representation of the temperature variations.

R STUDIO

RStudio is a free and open-source integrated development environment (IDE) for R, a programming language for statistical computing and graphics. RStudio was founded by JJ Allaire, creator of the programming language ColdFusion. Hadley Wickham is the Chief Scientist at RStudio. R Studio is available in two editions: RStudio Desktop, where the program is run locally as a regular desktop application; and RStudio Server, which allows accessing RStudio using a web browser while it is running on a remote Linux server. Prepackaged distributions of RStudio Desktop are available for Windows, macOS, and Linux. RStudio is available in open source and commercial editions and runs on the desktop (Windows, macOS, and Linux) or in a browser connected to RStudio Server RStudio is an awesome tool that can help you do your work better and faster. In technical terms, RStudio is a cross-platform integrated development environment for the R statistical language.

Cluster analysis : Cluster analysis or clustering[12] is the task of grouping a set of objects in such a way that objects in the same group (called a cluster) are more similar (in some sense or another) to each other than to those in other groups (clusters). It is a main task of exploratory data mining, and a common technique for statistical data analysis. It can be achieved by various algorithms that differ significantly in their notion of what constitutes a cluster and how to efficiently find them. Popular notions of clusters include groups with small distances among the cluster members, dense areas of the data space, intervals or particular statistical distributions. Clustering can therefore be formulated as a multi-objectiveoptimization problem. The appropriate clustering algorithm and parameter settings (includingvalues such as the distance function to use, a density threshold or the number of expected clusters) depend on the individual data set and intended use of the results.

Clustering in machine learning: Clustering: is the assignment of a set of observations into subsets (called clusters) so that observations in the same cluster are similar in some sense. Clustering is a method of unsupervised learning, and a common technique for statistical data analysis used in many fields.

Supervised and unsupervised learning in data mining

Supervised Learning[10] is the Data mining task of inferring a function from labelledtraining data. The training data consist of a set of training examples. In supervised learning, each example is a pair consisting of an input object (typically a vector) and a desired output value (also called the supervisory signal).

Unsupervised Learning[10] is a type of machine learning algorithm used to drawinferences from datasets consisting of input data without labelled responses. The most common unsupervised learning method is cluster analysis, which is used for exploratory data analysis to find hidden patterns or grouping in data.

Cluster in data mining: Cluster is a group of objects that belongs to the same class.In other words, similar objects are grouped in one cluster and dissimilar objects are grouped in another cluster.

K means clustering algorithm: K-means clustering [12] aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean, serving as a prototype of the cluster. This results in a partitioning of the data space into voronoi cells.

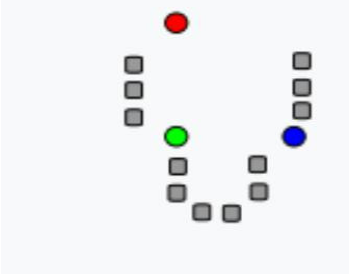
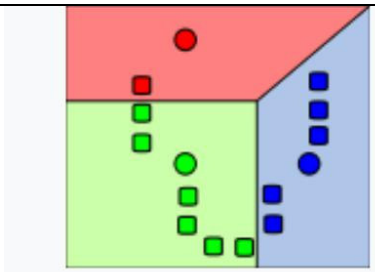
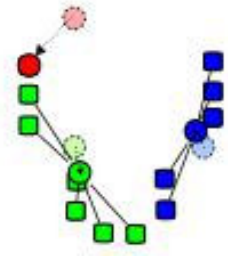
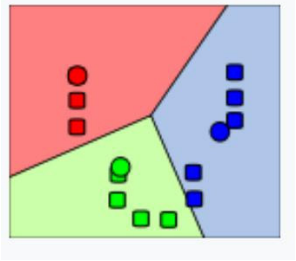
Working of k-means clustering algorithm : The input to K-Means is a set of points (observations), and an integer K. The goal is to partition the input points into K distinct sets (clusters). The first step is to initialize the algorithm by choosing K initial cluster centroid locations. ... These steps are repeated until the algorithm "converges".

Description : Given a set of observations (**x**1, **x**2, …, **x***n*), where each observation is a *d*-dimensional real vector, *k*-means clustering aims to partition the *n* observations into *k* (≤ *n*) sets **S** = {*S*1, *S*2, …, *Sk*} so as to minimize the within-cluster sum of squares (WCSS) (sum of distance functions of each point in the cluster to the K center).

INITIALIZATION METHODS

Commonly used initialization methods are Forgy and Random Partition.[7]The Forgy method randomly chooses *k* observations from the data set and uses these as the initial means. The Random Partition method first randomly assigns a cluster to each observation and then proceeds to the update step, thus computing the initial mean to be the centroid of the cluster's randomly assigned points. The Forgy method tends to spread the initial means out, while random Partition places all of them close to the center of the data set. According to Hamerly et al the Random Partition method is generally preferable for algorithms such as the *k*-harmonic means and fuzzy *k*-means. For expectation maximization and standard *k*-means algorithms, the Forgy method of initialization is preferable. A comprehensive study by Celebi et al.however, found that popular initialization methods such as Forgy, Random Partition, and Maximin often perform poorly, whereas the approach by Bradley and Fayyad performs "consistenty" in "the best group".

Demonstration of the standard algorithm

<table>
<tr><td>  </td><td>  </td><td>  </td></tr>
<tr><td>1. k initial "means" (in this case k=3) are randomly generated within the data domain (shown in color).</td><td>2. k clusters are created by associating every observation with the nearest mean. The partitions here represent the Voronoi diagram generated by the means.</td><td>3. The centroid of each of the k clusters becomes the new mean.</td></tr>
<tr><td></td><td> 
4. Steps 2 and 3 are repeated until convergence has been reached.</td><td></td></tr>
</table>

Value: k-means returns an object of class "k-means" which has a print and a fitted method. It is a list with at least the following components:

Cluster: A vector of integers (from 1:k) indicating the cluster to which each point is allocated.

Centers: A matrix of cluster centres.

Totss: The total sum of squares.

Withinss: Vector of within-cluster sum of squares, one component per cluster.

tot.withinss Total within-cluster sum of squares, i.e. sum (withinss).

Betweens: The between-cluster sum of squares, i.e. totss-tot.withinss.

Size: The number of points in each cluster.

Iter: The number of (outer) iterations.

Ifault: indicator of a possible algorithm problem – for experts.

SUMMARY

Requirements are R Language, Windows XP,7 , 8 Operating system, R, Rstudio, coolterm Technologies. Cool Term is a simple port terminal application that is geared towards hobbyists and professionals with a need to exchange data with hardware connected to serial ports such as servo controllers, GPS receivers, micro-controllers. A CSV is a comma separated values file which allows data to be saved in a table structured format. CSV look like a garden-variety spreadsheet but with a .csv extension. R is an implementation of the S programming language combined with lexicalscoping semantics inspired by Scheme. S was created by John Chambers while at Bell Labs. There are some important differences, but much of the code written for S runs unaltered.

In R, we can read data from files stored outside the R environment. We can also write data into files which will be stored and accessed by the operating system. R can read and write into various file formats like csv, excel, xml etc.
A line chart is a graph that connects a series of points by drawing line segments between them. The plot() function in R is used to create the line graph. Basic syntax plot(v, type, col, xlab, ylab). RStudio is a free and open-source integrated development environment (IDE) for R, a programming language for statistical computing and graphics. RStudio was founded by JJAllaire, creator of the programming language ColdFusion. Hadley Wickham is the Chief Scientist at RStudio. Cluster analysis or clustering is the task of grouping a set of objects in such a way that objects in the same group (called a cluster) are more similar (in some sense or another) to each other than to those in other groups. Supervisedlearning isthe Datamining taskofinferringa functionfrom labeled training data.The training data consist of a set of training examples. Unsupervised learning is a type of machine learning algorithm used to draw inferences from datasets consisting of input data without labelled responses. k-means clustering aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean, serving as a prototype of the cluster. This results in a partitioning of the data space into Voronoi cells.

RESULTS AND DISCUSSIONS

	A	B	C	D	E	F	G	H	I	J	K
1	id	diagnosis_result	radius	texture	perimeter	area	smoothness	compactness	symmetry	fractal_dimension	
2	1	M	23	12	151	954	0.143	0.278	0.242	0.079	
3	2	B	9	13	133	1326	0.143	0.079	0.181	0.057	
4	3	M	21	27	130	1203	0.125	0.16	0.207	0.06	
5	4	M	14	16	78	386	0.07	0.284	0.26	0.097	
6	5	M	9	19	135	1297	0.141	0.133	0.181	0.059	
7	6	B	25	25	83	477	0.128	0.17	0.209	0.076	
8	7	M	16	26	120	1040	0.095	0.109	0.179	0.057	
9	8	M	15	18	90	578	0.119	0.165	0.22	0.075	
10	9	M	19	24	88	520	0.127	0.193	0.235	0.074	
11	10	M	25	11	84	476	0.119	0.24	0.203	0.082	
12	11	M	24	21	103	798	0.082	0.067	0.153	0.057	
13	12	M	17	15	104	781	0.097	0.129	0.184	0.061	
14	13	B	14	15	132	1123	0.097	0.246	0.24	0.078	
15	14	M	12	22	104	783	0.084	0.1	0.185	0.053	
16	15	M	12	13	94	578	0.113	0.229	0.207	0.077	
17	16	M	22	19	97	659	0.114	0.16	0.23	0.071	
18	17	M	10	16	95	685	0.099	0.072	0.159	0.059	
19	18	M	15	14	108	799	0.117	0.202	0.216	0.074	
20	19	M	20	14	130	1260	0.098	0.103	0.158	0.054	

Prostate_Cancer

Fig 1: Data Set

```
> setwd("C:/Users/Payal/Desktop/KNN")
> prc <- read.csv("Prostrate_Cancer.csv",stringsAsFactors = FALSE)
> str(prc)
'data.frame':   100 obs. of  10 variables:
 $ id                : int  1 2 3 4 5 6 7 8 9 10 ...
 $ diagnosis_result  : chr  "M" "B" "M" "M" ...
 $ radius            : int  23 9 21 14 9 25 16 15 19 25 ...
 $ texture           : int  12 13 27 16 19 25 26 18 24 11 ...
 $ perimeter         : int  151 133 130 78 135 83 120 90 88 84 ...
 $ area              : int  954 1326 1203 386 1297 477 1040 578 520 476 ...
 $ smoothness        : num  0.143 0.143 0.125 0.07 0.141 0.128 0.095 0.119 0.127 0.119 ...
 $ compactness       : num  0.278 0.079 0.16 0.284 0.133 0.17 0.109 0.165 0.193 0.24 ...
 $ symmetry          : num  0.242 0.181 0.207 0.26 0.181 0.209 0.179 0.22 0.235 0.203 ...
 $ fractal_dimension: num  0.079 0.057 0.06 0.097 0.059 0.076 0.057 0.075 0.074 0.082 ...
>
```

Fig 2: Reading the value

```
   Cell Contents
|-------------------------|
|                       N |
|           N / Row Total |
|           N / Col Total |
|         N / Table Total |
|-------------------------|

Total Observations in Table:  35

                 | prc_test_pred
prc_test_labels  |         B |         M | Row Total |
-----------------|-----------|-----------|-----------|
               B |         5 |        14 |        19 |
                 |     0.263 |     0.737 |     0.543 |
                 |     1.000 |     0.467 |           |
                 |     0.143 |     0.400 |           |
-----------------|-----------|-----------|-----------|
               M |         0 |        16 |        16 |
                 |     0.000 |     1.000 |     0.457 |
                 |     0.000 |     0.533 |           |
                 |     0.000 |     0.457 |           |
-----------------|-----------|-----------|-----------|
    Column Total |         5 |        30 |        35 |
                 |     0.143 |     0.857 |           |
-----------------|-----------|-----------|-----------|
```

Fig 3: Normalizing function

```
> normalize <- function(x) {
+  return ((x - min(x)) / (max(x) - min(x)))
+  }
> prc_n <- as.data.frame(lapply(prc[2:9], normalize))
> summary(prc_n$radius)
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
 0.0000  0.1875  0.5000  0.4906  0.7500  1.0000
>
```

Fig 4: Training models

```
>  prc_train <- prc_n[1:65, ]
>  prc_test <- prc_n[66:100, ]
> prc_test_labels <- prc[66:100, 1]
> prc_train_labels <- prc[1:65, 1]
> prc_test_labels <- prc[66:100, 1]
> prc_test_pred <- knn(train = prc_train, test = prc_test,cl = prc_train_labels, k=10)
Error: could not find function "knn"
> install.packages("class")
Installing package into 'C:/Users/Payal/Documents/R/win-library/3.1'
(as 'lib' is unspecified)
--- Please select a CRAN mirror for use in this session ---
trying URL 'http://mirrors.xmu.edu.cn/CRAN/bin/windows/contrib/3.1/class_7.3-13.zip'
Content type 'application/zip' length 100211 bytes (97 Kb)
opened URL
downloaded 97 Kb

package 'class' successfully unpacked and MD5 sums checked

The downloaded binary packages are in
        C:\Users\Payal\AppData\Local\Temp\RtmpkPNcE8\downloaded_packages
> library(class)
```

Fig 5: Output form

CONCLUSION AND FUTURE WORK

Big Data is used in predictive analysis and decision making in companies with wide number of services. The ever growing information has started growing exponentially recently and Big Data is the only technology that can help us in making the best use of this data. The companies are investing and working hard on developing the algorithms for better usage of this technology. It can be embedded with various technologies like IOT, decision making, clustering. The decision making process is totally revolutionized by the implementation of Big Data. Various companies are already using the analysis techniques of Big Data to research the information and make the decisions for long future. It can be said that Big Data is the only scope for using the resources of information in near future. It is no exaggeration to say that this is the only technology that prevails as long as the use of information stays.

Future Scope: Big Data is making its mark in the fields that use information as the powerful resource. It is estimated that Big Data is going to accommodate 1,90,000 data scientists and 1.5 Million managers by 2018. Big Data analytics is a top priority by lot of organizations. It provides 45% more accurate predictions and business insights.

Sangram Keshari Swain

Big Data analytics provides an edge over competition, the rate of implementation of the analytics tools has increased exponentially. The apache Hadoop framework is one of the most used big data frameworks. It fulfills the requirement of commercial and open source frameworks to choose from organizations and make appropriate choice. Data analytics is a key factor in decision making for future. 96% of the organizations feel that analytics is the key source to make decision in the future of their organization for the next three years.

REFERENCES

1. 1.Big Data: Issues, Challenges, Tools and Good practices produced by Avita Katal, Mohammad Wazid, R.H. Goudar
2. Big Data: Issues and challenges moving forward produced byStephen kaisler, Frank Armour, J. Alberto Espinosa, William Money
3. 3.Big Data computing computing and clouds: Trends and future directions produced by Marcos D. Assuncao, Rodrigo N. Calheiros, Silvia Bianchi, Marco A.S. Netto, Rajkumar Buyya.

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RESEARCH ARTICLE

IoT Based Industrial Automation Control

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ABSTRACT

In the simplest terms, the Internet of Things (IoT) is how we describe the digitally connected universe of everyday physical devices. These devices are embedded with internet connectivity, sensors and other hardware that allow communication and control via the web. IoT makes once "dumb" devices "smarter" by giving them the ability to send data over the internet, allowing the device to communicate with people and other IoT-enabled things It's difficult to imagine the world without advancement in technology implementation. Now IOT is taking up the industry.Industrial Automation field is now in the era of fastdeveloping industry. It is now well known as IIOT by adding IoT to the industrial automation. Now the latest development is IIoT 4.0.

Keywords: Internet of Thing (IoT), Programmable Logic Controller (PLC), Supervisory Control And Data Acquisition (SCADA).

INTRODUCTION

IIoT is a concept where industrial automation is combined with IoT in process control. The industrial internet of things (IIoT) is the use of smart sensors and actuators to enhance manufacturing and industrial processes. Also known as the industrial internet or Industry 4.0, IIoT leverages the power of smart machines and real-time analytics to take advantage of the data that dumb machines have produced in industrial settings for years. Although the internet of things and the industrial internet of things have many technologies in common, including cloud platforms, sensors, connectivity, machine-to-machine communications and data analytics, they are used for different purposes. IoT applications connect devices across multiple verticals, including agriculture, healthcare, enterprise, consumer and utilities, as well as government and cities. IoT devices include smart appliances, fitness bands and other applications that generally don't create emergency situations if something goes amiss.

IIoT applications, on the other hand, connect machines and devices in such industries as oil and gas, utilities and manufacturing. System failures and downtime in IIoT deployments can result in high-risk situations or even life-threatening situations. IIoT applications are also more concerned with improving efficiency and improving health or safety, versus the user-centric nature of IoT applications. The driving philosophy behind IIoT is that smart machines are not only better than humans at capturing and analysing data in real time, they are better at communicating important information that can be used to drive business decisions faster and more accurately.

IOT BASED INDUSTRIAL AUTOMATION CONTROL

In this we have tried a process control using IIoT, PLC and SCADA. The process was to purify and destalinization of milk in three containers. The process was controlled by PLC and the visualization was made on SCADA for monitoring and control. Some of the PLC controls are controlled by the help of IoT. One of the IoT (work as switching device) kept at Cuttack, city in Odisha and the second IoT is kept at Centurion University of Technology & Management, Jatni, Khurda, in Odisha itself, both the places are 50 Km apart from each other. Both IoT's are on different network worked fine for switching and controlling the PLC. The IoT at Cuttack was programmed to trigger the PLC process and some other variable controls and the same time the second IoT at Jatni receives the signal and feed to Arduino. Arduino process the signal and that processed signal is feed to PLC for controlling the Process. Architecture, standards and data processing. Figure 1 : Testing setup of the Process. This application can be utilized in different applications as shown in the figure 2.

RESULT AND ANALYSIS

The setup made as per the above diagram and a test has been activated. The principle of the test is to activate the process. So a signal from the IoT one is generated and then the signal is received at second IoT which is connected to an Arduino. The output of Arduino is feed to PLC. Then the ladder logic of PLC activates the process and a SCADA displays the total process on the computer screen. The test run was satisfactory and the operation of the process started and executed as per the parameters.

CONCLUSION

This paper provides an in-depth literature review of basic IIoT application which is carried out with a test done with the help of IoT, PLC and SCADA. We had tried to control a milk process system with IoT. The future aspects are flourishing now a days and the future industries will IIoT based and known as Industry 4.0.

REFERENCES

1. [online] Available: http://www.intemet-of-things- research.eu/ pdf/IERCClusterBook2012_WEB.pdf.
2. Piero Fraternali, Gustavo Rossi, Fernando Sánchez-Figueroa, "Rich Internet Applications", *IEEE Internet Computing*, vol. 14, no. 3, pp. 9-12, May/June 2010.
3. *Delta AH-500 PLC module reference*, [online] Available: http://www.ferret.com.au/ ODIN/PDF/ Showcases/105517.pdf.
4. [online] Available: http://www.aps.anl.gov/epics/.
5. *Pymodbus Python Package*, [online] Available: https://pypi.python.org/pypi/pymodbus.
6. [online] Available: http://en.wikipedia.org/wiki/Smart_city#Examples_of_use.

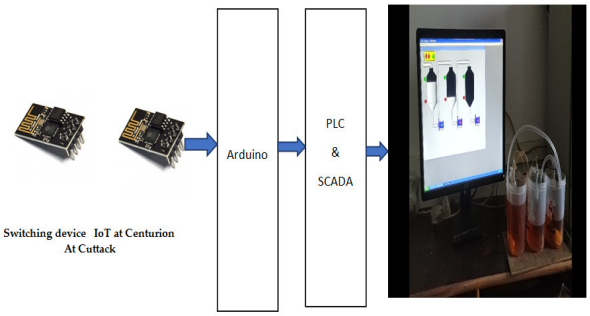

Figure 1 : Testing setup of the Process

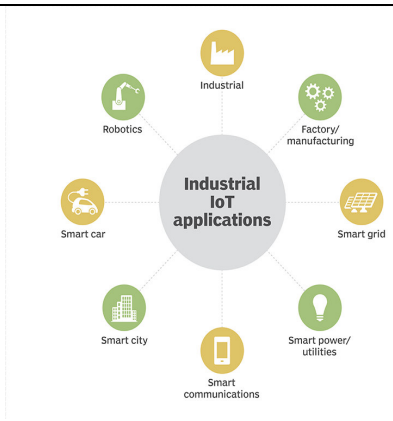

Figure 2: Different application IIoT

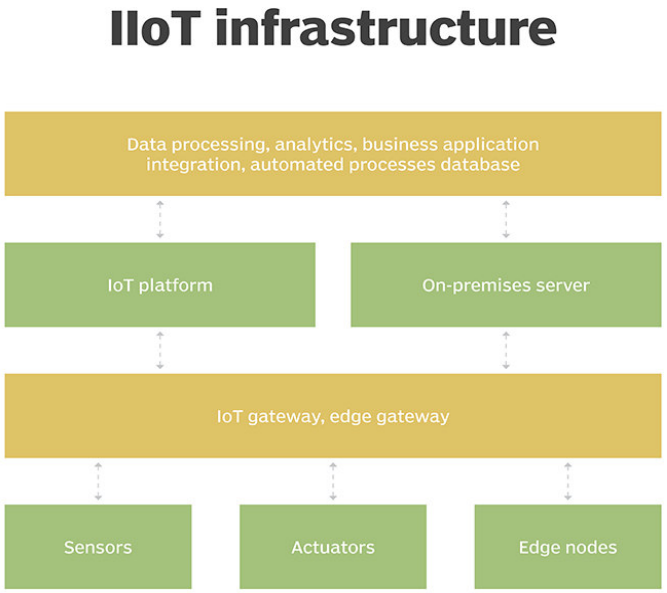

Figure 3 : Future scope of IIoT

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RESEARCH ARTICLE

Python Based Data Presentation of Industrial Automation

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ABSTRACT

A set of predefined jobs executed sequentially and systematically by the help of hardware and software is the concept of industrial automation. Industrial automation helps in Increasing Productivity, Increasing Quality, Reducing Cost, Increasing Safety in working conditions. Industrial automation is basically consisting of Hardware control, Software control and Field instruments. Hardware control is consisting of microcontrollers, PID controllers, PLC controllers and DCS controllers. Software controller is SCADA and field instruments is consists of sensors and output devices. Python is an interpreted, object-oriented, high-level programming language with dynamic semantics. Python's simple, easy to learn syntax emphasizes readability and therefore reduces the cost of program maintenance. Python supports modules and packages, which encourages program modularity and code reuse.

Keywords: Programmable Logic Controller (PLC), Supervisory Control and Data Acquisition (SCADA).

INTRODUCTION

Python turns out to be surprisingly versatile in this setting, whether for prototyping a single conveyor belt or taming a building full of robots. This talk explains how to use Python for interfacing with two common industrial automation devices: a barcode scanner and a Programmable Logic Controller (PLC). The only thing we have used Python for recently was to take a PLC database and translate it into a bunch of EXCEL files. It is better in my opinion to work on something other than the working database to get those translations right or sensible. One advantage that we did realize a bit afterwards is that we can store additional data in these files such as data on field devices, calibration info and set points. As such,kind of wish that we had used python to port the comma separated database to some sort of relational database. It is actually a good example of the power of Python and the associated libraries.

Python based data presentation of Industrial Automation

Basic principle: Here we have tried get a temp sensor parameter dipped in a fluid in side a container. The container is then heated with a help of a heater. The sensor is connected to the PLC input card and heater is connected to the PLC output card. In the PLC we have written a ladder diagram to get the temperature sensor data ant to control the heater. A SCADA design and program is written inside the SCADA software, which will display the temperature data on the screen. Then this data is feed to a EXCEl file by using DAT BASE CONNECTIVITY property inside the SCADA. So the change in temperature will be displayed in PLC, SCADA and EXCEL simultaneously. The temperature data will be then fetched from EXCEL file to PYTHON software. Python software will display the data in a graphical representation format. The program of Python is shown below for reference

Python program

```
import xlrd
import matplotlib.pyplot as plt
sheet=xlrd.open_workbook ("E:/python/Test/demand1.xlsx").sheet_by_index(0)
times=[]
temps=[]
for row in range(0,5):
time = sheet.cell_value((row+1),0)
temp = sheet.cell_value((row+1),1)
times.append(time)
temps.append(temp)

plt.plot(times,temps)
plt.title(" Time Vs Temperature ")
plt.xlabel(" times ")
plt.ylabel(" temps ")
#plt.xlim(20,60)
plt.show()
```

Figure 1: Program of Python

Architecture, standards and data processing

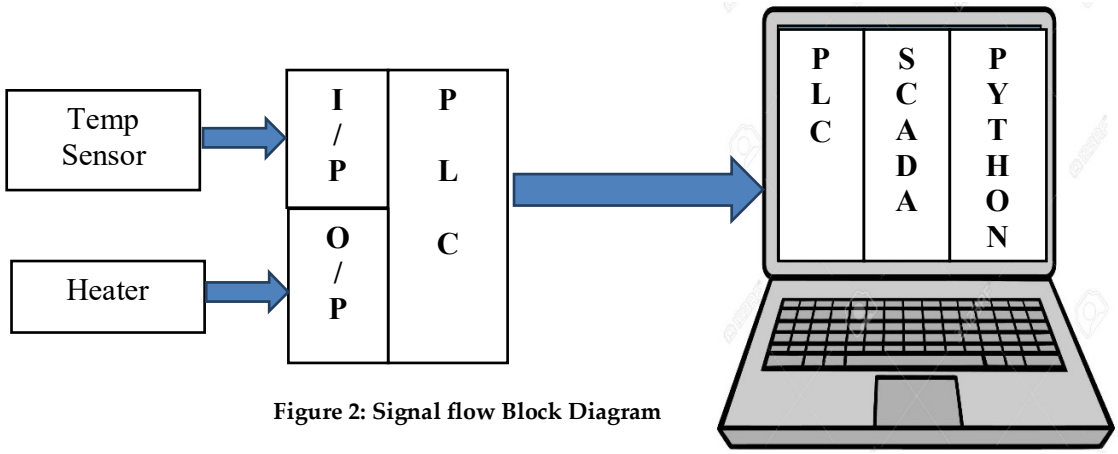

Figure 2: Signal flow Block Diagram

Application Python based data presentation of Industrial Automation

- Python can be use with Industrial Automation for display the data in 3D or 4D graph pattern
- It can be used for predictions of faults.
- It can be used for huge data storage.
- It can be used for the process control and estimation and costing of the product, time, quality, etc.

RESULT AND ANALYSIS

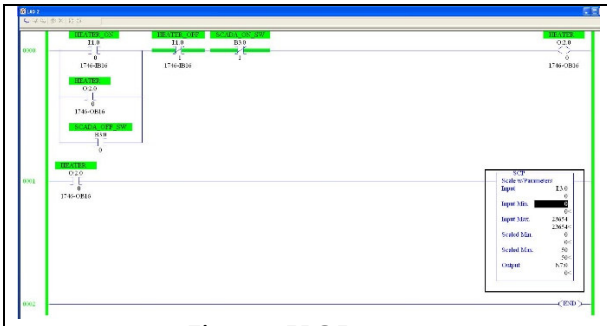

Figure 3: PLC Program

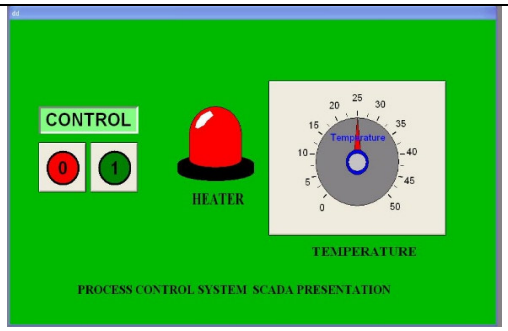

Figure 4: SCADA Visualization

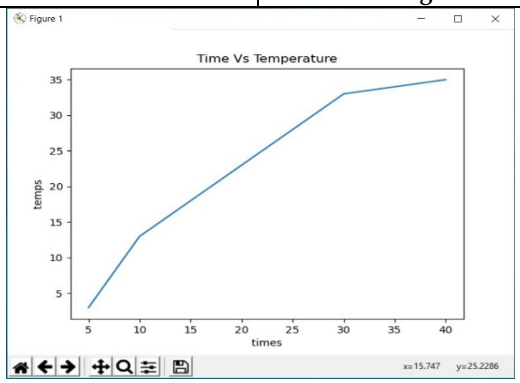

Figure 3: Python Program output

CONCLUSION

We presented this paper to introduced the concept of a system in which smart sensors were applied to monitor and control the various industrial parameters. The temperature sensor output is scaled inside the PLC which is calculated and then SCADA gets the datafor presentation as well as the data is feed to excel and we get the desired value in the EXCEL. Then the Data is processed as per requirement of Python and the output is presented in the format of graph.

REFERENCES

1. Ahmad Rabie, Mare Hanheide, Modesto Castrillion Santana "Automatic Initialization for Facial Analysis in Interactive Robotics" journal of "Bielefeld University, Germany & University of Las Palmas de Gran Canaria, Spain, 2008.
2. Balkeshwar Singh. "Role of Industrial Robots in Lean Manufacturing System" journal of "International Journal of Scientific Research Engineering & Technology (IJSRET)" vol.1, issue 3, pp150-153, August 2012.

3. Balkeshwar Singh, Kumara Dhas, "Evolution of Industrial Robots and their Applications" journal of "International Journal of Scientific Research Engineering & Technology and Advanced Engineering (IJETAE)" vol.3, issue 5, May 2013.
4. David Durocher, Senior Member IEEE Arc-flash Compliance Implementations at Industrial Processing Facilities IEEE Transactions on Industry Applications, vol.51, no.2, Mar/Apr 2015.
5. Douglas Blank, Lisa Meeden and Holly Yanco, "Pyro: An Integrated Environment for Robotics Education" journal of

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RESEARCH ARTICLE

Smart Substation with Dashboard

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ABSTRACT

Electrical power systems are a technical wonder. Electricity and its accessibility are the greatest engineering achievements of the 20th century. A modern society cannot exist without electricity. Generating stations, transmission lines and distribution systems are the main components of power system. Smaller power systems (called regional grids) are interconnected to form a larger network called national grid, in which power is exchanged between different areas depending upon surplus and deficiency. This requires a knowledge of load flows, which is impossible without meticulous planning and monitoring. Also, the system needs to operate in such a way that the losses and in turn the cost of production are minimum. The major factors that influence the operation of a power system are the changes in load and stability. As is easily understood from the different load curves and load duration curve, the connected load, load varies widely throughout the day. These changes have an impact on the stability of power system. As a severe change in a short span can even lead to loss of synchronism. Stability is also affected by the occurrence of faults. Faults need to be intercepted at an easily stage and corrective measures like isolating the faulty line must be taken. As the power consumption increases globally, unprecedented challenges are being faced, which require modern, sophisticated methods to counter them. This calls for the use of automation in the power system. The Supervisory Control and Data Acquisition (SCADA) and Programmable Logic Controllers (PLC) are an answer to this. SCADA refers to a system that enables on electricity utility to remotely monitor, co-ordinate, control and operate transmission and distribution components, equipment and real-time mode from a remote location with acquisition at date for analysis and planning from one control location. PLC on the other hand is like the brain of the system with the joint operation of the SCADA and the PLC, it is possible to control and operate the power system remotely. Task like opening of circuit breakers, changing transformer taps and managing the load demand can be carried out efficiently. This type of an automatic network can manage load, maintain quality, detect theft of electricity and tempering of meters. It gives the operator an overall

view of the entire network. Also, flow of power can be closely scrutinized and Pilferage points can be located. Human errors leading to tripping can be eliminated. This directly increases the reliability and lowers the operating cost.

Keywords: Current transformer (CT), Potential transformer (PT), Programmable Logic Controller (PLC), Supervisory Control and Data Acquisition (SCADA), Zero Crossing Detection (ZCD).

INTRODUCTION

The digital substation is a term applied to electrical substations where operation is managed between distributed intelligent electronic devices (IEDs) interconnected by communications network. Due to overloading conductors are brakes at any time in the substation which is very harmful for substation and their worker's security. SCADA is used for monitoring the voltage, current, power &. frequency in a substation and to protect the system from the rise in mentioned parameter on real time basis, in order to enhance the controlling during fault condition, efficiency of substation, all equipment's are converted into modern technology i.e. SCADA technology. All old equipment's are controlled and monitored by using SCADA. The system is accomplished by using PLC ladder diagram and SCADA software. In this project a step-down distributed substation is well monitored and controlled by PLC and SCADA as a prelude to substation automation. PLC plays crucial role in automation acting as a controller while SCADA act as a interfacing medium.

Electrical Dashboard Technology

Basic Principle

Substations are a critical component for maintaining electrical supply and load control in low voltage, medium voltage and high voltage electrical distribution networks. In order to ensure the proper functioning of substations and related equipment such as line-mounted switches and capacitors. The basic components for this system are CT, PT works as an input to PLC. These inputs give raw data to PLC which are scaled into the required range. Then a ladder logic program is written and a graphical presentation is made by the help of SCADA. Both the software (PLC & SCADA) work simultaneously to visualize and control the substation.

Current Transformer (CT)

A current transformer has a primary winding, a core and a secondary winding, although some transformers, including current transformers, use an air core. While the physical principles are the same, the details of a "current" transformer compared with a "voltage" transformer will differ owing to different requirements of the application. A current transformer is designed to maintain an accurate ratio between the currents in its primary and secondary circuits over a defined range. Split-core current transformers either have a two-part core or a core with a removable section. This allows the transformer to be placed around a conductor without having to disconnect it first. Split-core current transformers are typically used in low current measuring instruments, often portable, battery-operated, and hand-held.

Potential Transformer (PT)

The potential transformer may be defined as an instrument transformer used for the transformation of voltage from a higher value to the lower value. This transformer step down the voltage to a safe limit value which can be easily measured by the ordinary low voltage instrument like a voltmeter, wattmeter and watt-hour meters, etc. A zero-crossing detector or ZCD is one type of voltage comparator, used to detect a sine waveform transition from positive and negative, that coincides when the i/p crosses the zero-voltage condition. The applications of the Zero Crossing Detector are phase meter and time marker generator.

PLC & SCADA

Programmable Logic Controller is an electronic controller. Which is capable of handling analog signal (0volt to 10 volt and 4 milli ampere to 20 milli ampere) and digital signal (24 volt dc). It is programmed with different programming styles in which ladder logic is in common. Supervisory Control And Data Acquisition (SCADA) is a software controller which takes sensor parameters from the field, factory and industries through PLC to the central computer from monitoring and control. It is a software controller but not a 100% controller.

Architecture, standards and data processing

Circuit architecture

What we have tried is taking the signals from the substation through the CT, PT and ZCD to the PLC for different processing and calculation. These data's are then send to SCADA for visualization and control. By using ladder program and SCADA software we can monitor the different parameters of the substation. By getting these parameters we can activate alarms for different operations like over voltage, over current, over frequency, unbalanced load distribution, earth failure etc. By the help of these data even we can control the above faulty operations.

Measurement layer

Measurement layer consists of current transformers (CTs), potential transformers (PTs), zero crossing detection, PLC and SCADA. The process data by the help of PLC & SCADA are used to monitor and control the substation.

Application of the smart substation with dashboard.

It can be used to any substation. It can be implemented wherever there is a substation or power house or distribution centre is in operation by simple and small modification.

- Hydro power station.
- Thermal power station
- Solar power station
- Micro grid
- Substations

RESULT AND ANALYSIS

By the above description of circuit and working principal we have come to the final output. Which was satisfactory and tested ok. The output result is described above with a circuit and its operation. Here the frequency data was gathered by the help of zero detection circuit which has to be calibrated as per the circuit requirement. This device can be implemented by any service provider to trace fault before any shutdown due to error. It can activate alarms before any burn-out of any device. Now we are adding PLCC technology to it for better and a bit less cost effectiveness.

CONCLUSION

This paper provides an in-depth literature review of Smart substation with dash board its architecture, placement techniques and applications in distribution systems. The review also presents potential research areas techniques and Smart substation with dash applications in distribution systems. PLC and SCADA are deployed in large number in distribution networks but with the addition of more Smart substation with dash board resources, they are will become popular in the distribution system. Most of the applications presented in this paper are currently in testing mode to be useful in the electric power industry. These applications use data analytics and machine learning algorithms for power systems fault and detection. With Smart substation with dash board, the benefits gained in

terms of reliability, resiliency and operational efficiency of the grid justifies its instalment. It is expected that with further proliferation of data resources Smart substation with dash boardcan perform many of the aforementioned tasks with more accuracy and reliability.

REFERENCES

1. Zhenya Liu, the Technology of Smart Grid, CEPP, 2010.
2. Wenliang Zhang, Zhuangzhi Liu, Mingjun Wang, et al. "Research status and development trend of smart grid," Power System Technology, 2009, 33(13): 1-11.
3. Yixin Yu, and Wenpeng Luan, "Smart grid and its implementations," Proceedings of the CSEE, 2009, 29(43): 1-8.
4. Technical Guide for Smart Substation, State Grid Company Standard, CQ/GDW 383-2009.
5. Specifications of design for 110(66) kV~220kV Smart Substation, State Grid Company Standard, CQ/GDW 393-2009.
6. Specifications of design for 330kV~750kV Smart Substation, State Grid Company Standard, CQ/GDW 394-2009.
7. Technical Guide for Smart Electric Equipments, State Grid Company Standard, Q/GDW Z 410-2010.
8. Technical Specification of Protection for Smart Substation, State Grid Company Standard, Q/GDW 441- 2010.
9. The Technical Specification for Electronic Current Transformers, State Grid Company Standard, Q/GDW 424-2010.
10. Supplementary Regulations for New Substation Design in 2011, State Grid Company, [2011] 58.
11. Suggestion of Optimally Integrated design and construction for Smart Substation, State Grid Company, [2011] 539.
12. Technical Guide for Online Monitoring System of Substation Equipments, State Grid Company Standard, Q/GDW 534- 2010.

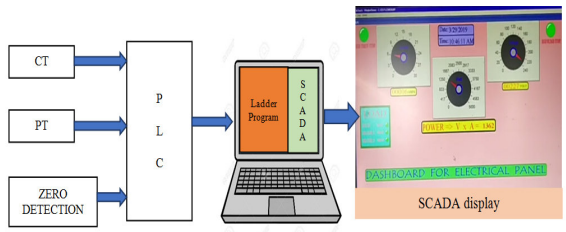

Figure 1 : Functional block Diagram

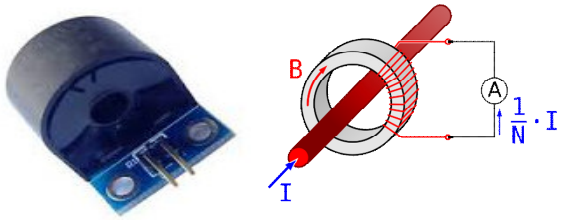

Figure 2 : Current transformer

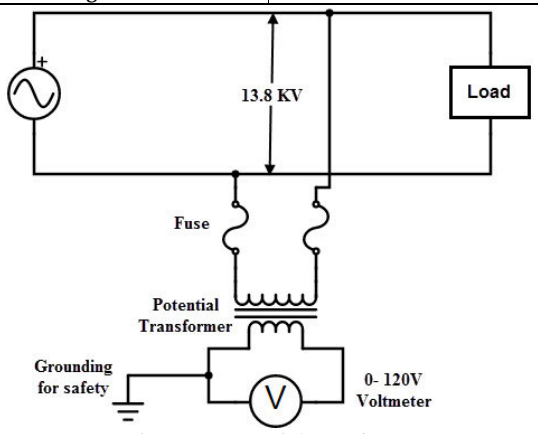

Figure 3 : Potential transformer

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RESEARCH ARTICLE

Maintenance Problem in Automation and its Related Solution to Them in Industry

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ABSTRACT

The current society has the advanced technology with them. If the machines are working or performing a task, means there is always something that drives or guides them. With the advent of various PLCs, SCADA, HMI and Drives, the operation of motors have become smooth and more efficient. The power system comprises of generating stations, transmission lines and distribution systems. From the distribution sytems, the various industries gets electrical energy. The industries like manufacturing, packaging, shipping, agriculture, healthcare etc use the modern sophisticated machines and tools for increasing the accuracy, productivity and efficiency of the system. Also, the system needs to operate in such a way that the losses and in turn the cost of production are minimum. The major factors that influence the operation of an industry are the changes in load and stability. As is easily understood from the different load curves and load duration curve, the connected load, load varies widely throughout the day. As a result requirement of power is also for different times. Then comes the various kinds of faults in an industry. But one thing is important that the faults need to be intercepted at an early stage and corrective measures like isolating the faulty line must be taken. As the requirement of power increases across the globe, unprecedented challenges are being faced, which require modern, sophisticated methods to counter them. Here is the part where automation comes into picture. The Supervisory Control and Data Acquisition (SCADA) and Programmable Logic Controllers (PLC) are the befitting answer to these challenges. SCADA refers to a system that enables on electricity utility to remotely monitor, co-ordinate, control and operate transmission and distribution components, equipment and real-time mode from a remote location with acquisition at date for analysis and planning from one control location. PLC on the other hand is like the brain of the system with the joint operation of the SCADA and the PLC, it is possible to control and operate the power system remotely. Task like opening of circuit breakers, changing transformer taps and managing the load demand can be carried out

efficiently. This type of an automatic network can manage load, maintain quality, detect theft of electricity and tempering of meters. It gives the operator an overall view of the entire network. Human errors leading to tripping can be eliminated. This minimizes the operating cost there by increasing the productivity.

Keywords: Proximity sensors, Normally Open(NO type), Normally Closed (NC type), Programmable Logic Controller (PLC), Supervisory Control And Data Acquisition (SCADA),Miniature Circuit Breaker(MCB).

INTRODUCTION

Automation is the way of generating and using technology to look into and channelize processes that can develop and generates products and services. This method uses the three basic principles of measurement, control, and action. When it comes to design, monitor and develop, skilled operators and engineers follow the path of automation, it means the problems are attended and the solutions are provided aptly. Skilled persons have to learn all the stages of an automated process and all such processes need both knowledge and applicability skill, across all the engineering branches. As automation leverage the industrial plants output more efficiently, so there is a need of updating the automation systems and process the maintenance periodically by skilful labours. Previously maintenance could only happen when a service person was physically present, but with the advent of technology and different skill development programs the technicians are allowed to learn and practice their skills towards success in these periodically maintained schedules. Today the availability of efficient and much reliable network systems have enabled the technology to reach the remote areas and also have enabled quality service in those areas. The problems are solved using latest and sophisticated technology. In this report it has been explained the maintenance problem in industry and the adequate steps taken to counter them. Many a problems arise and the necessary and timely steps are taken to take care of them.

ABOUT AUTOMATION MAINTENANCE ISSUES

Previously the manual data collection was time consuming and in turn was taking the maintenance time. Additionally, a skilled set of people is necessary to operate and so the maintenance issues. They should possess the fundamentals of controlling knowledge, knowledge of electrical and process equipment, and detailed process understanding. Howsoever large the automation system is, but they need human assistance to get themselves out of the critical problems. Human intervention is required. Automation systems comprises of hard drives, controllers, monitors, jumpers, firmware, software, and hardware. For example if a simple fan is ignored, a controller can overheat and result in a portion of a plant being shut down. In many organizations there are fewer trained personnel to perform maintenance. I had recently visited an industry Prasad Seeds Private Limited, Medchal, Telengana, which was concerned of their automation systems maintenance and were providing the expected levels maintenance so that the automation system can run smoothly for longer days to come. Below mentioned are some of the problems observed and the necessary solutions given to the automation system in the industry.

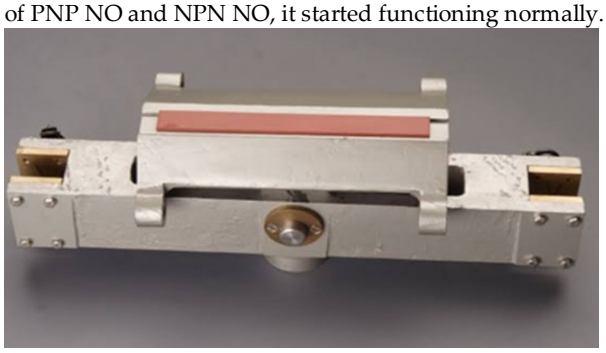
Problem

When the Nichrome Machine Horizontal Jaw doesn't work systematically:

- Proximity sensor's faulty operations.
- Proximity sensor doesn't turn ON/OFF.

Solutions

PNP and NPN sensors are both supplied with positive and negative power leads, then they produce a signal to indicate an 'ON' state. PNP sensor produces a positive output to industrial controls input, while NPN sensor produces a negative signal during an "ON" state. There are two types of sensors like PNP NO type and NPN NC type used near the NICHROME machine. If the NICHROME jaw is operated, then two numbers of PNP NO give the positive signal whereas NPN NO gives the negative signal during an ON state. But in the industry only one PNP NO and one NPN NO was used. As a result the sensor wasn't turning ON & OFF sequentially and no signal was found across the Nichrome horizontal jaw. So, in this condition the horizontal jaw fails to work. By applying two numbers of PNP NO and NPN NO, it started functioning normally.



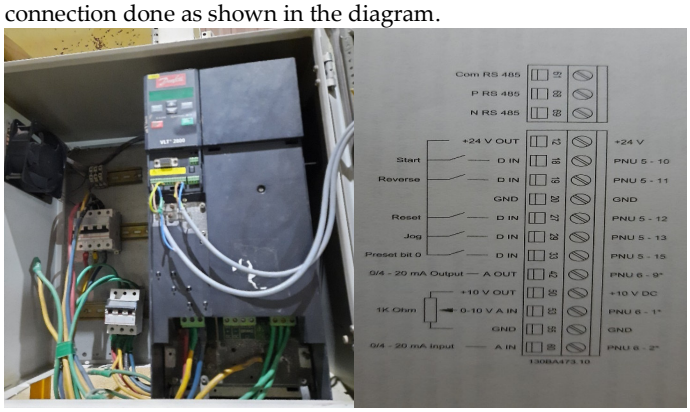
Problem

When DANFOSS VLT 2800 Drive gives error signal like: -

- Sending warning signal and alarm message.
- Showing two numbers in message that is 4 & 8.

Solutions

While the technician checks the drive, if it shows two messages with warning signal that is 4 & 8 numeric number. Then it's concluded that these are the error signal. That guide(manual) shows- number 4 indicates that there is no phase on mains supply side and number 8 shows the intermediate voltage is lower than the voltage set. So first the driver input voltage is checked using multi-meter which shows that a single-phase supply is not coming out of the three phase supply. Then the mains of MCB that is the 63 amps rating is checked, and found that the MCB was not properly working. There was no link between from input side to output side of the MCB. So, a new MCB of 63 amps was connected. After connecting MCB, the mains were made ON. But the system again was showing the number 45 error signal. This number indicates that the internal fault in Danfoss driver. So the driver unit was replaced and connection done as shown in the diagram.



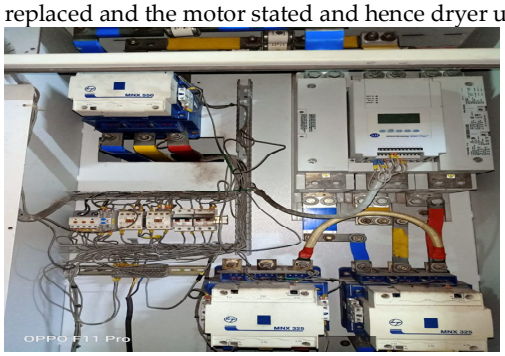
Problem

Dryer – 2 Unit Fails To Start: -

- Two 300 HP motor don't start.
- Four blowers don't get start.
- Contactor fails to start

SOLUTIONS

At starting the technician couldn't get any solution after searching all parameter in control panel, motor panel, bus - bar unit etc. The incoming and outgoing voltages in busbar panel were checked, but it also showed everything was ok. Then measurement panel was checked where current transformer is connected to busbar that showed how much current was flowing inside the busbar. It was showing the rated current flowing through it. At last when the electrical contactor was checked, it was found that the fault was inside the contactor. The contactor had failed to start, because the contactor was directly connected with 300 HP motor which takes 800 amps current. When the contactor was operated or made ON/OFF, the contactor choked and failed to carry current. So, the contactor unit was replaced and the motor stated and hence dryer unit started operating normally.



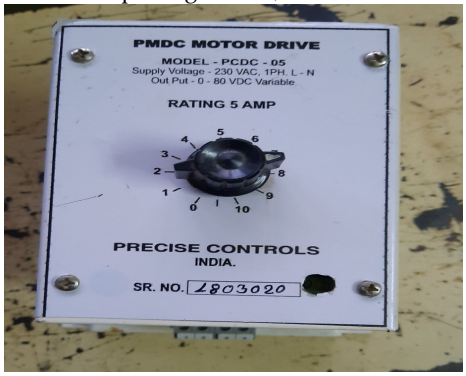
Problem

PMDC Motor Drive Fault

- PMDC Motor driver short circuits/becomes direct.
- After shorting the PMDC drive, the fuse blows out.
- After fusing the fuse element of the driver, the motor continuously runs, and it could not be stopped.

Solutions

- The PMDC motor drive was replaced.
- Fuse was also replaced.
- After replacing PMDC, its value was set 24 volt and finally the dc motor started running normally.



Problem

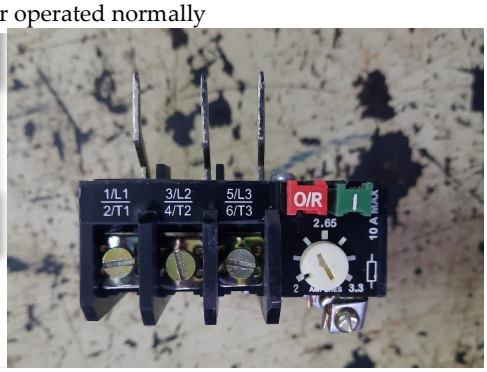
Phase Sequencer & Relay Fault: -

Motor doesn't start.

Relay's NC doesn't work.

Solutions

When it was found that a motor was not starting, first using multi-meter it was checked how much current & voltage was present in each phase of the main MCB. It showed the required values on each single phase. When the phase sequencer was checked, it was found that all phase voltages were not as per requirement because one of the phases was short circuited, so different voltages were showing in each phase. This problem was resolved by changing the phase sequence indicator and the motor started running smoothly. After the starting of the motor it was found that even if the fault or over load current flows still the relay's NC switch was not operating or tripping. Finally the relay was changed and the motor operated normally



RESULT AND ANALYSIS

By the above description of different faults in an automated industry and implementing different methods of trouble shooting, it was tested ok. The different trouble shooting methods were monitored after the restoration work. The characteristics of the present functioning of different equipments were exactly the similar like the desired way previously.

CONCLUSION

This paper provides an in-depth literature review of Maintenance Problem in Automation and It's Related Solution to Them in Industry. The review also presents potential research areas techniques and Maintenance Problem in Automation and It's Related Solution to Them in Industry applications in different automated systems. PLC and SCADA are deployed in large number in automated and various distribution networks but it is necessary to have regular maintenance and checking to prevent unnecessary brakedown of the field instruments resulting in the stopping of the industrial works. Most of the applications presented in this paper are currently being implemented to be useful in the electric power industry. It is expected that with further problems in the industries the paper can be upgraded so that many of the aforementioned problems and the future problems can be dealt with more accuracy and reliability.

REFERENCES

1. Zhenya Liu, the Technology of Smart Grid, CEPP, 2010.

2. Wenliang Zhang, Zhuangzhi Liu, Mingjun Wang, et al. "Research status and development trend of smart grid," Power System Technology, 2009, 33(13): 1-11.
3. Yixin Yu, and Wenpeng Luan, "Smart grid and its implementations," Proceedings of the CSEE, 2009, 29(43): 1-8.
4. Technical Guide for Smart Substation, State Grid Company Standard, CQ/GDW 383-2009.
5. Specifications of design for 110(66) kV~220kV Smart Substation, State Grid Company Standard, CQ/GDW 393-2009.
6. Specifications of design for 330kV~750kV Smart Substation, State Grid Company Standard, CQ/GDW 394-2009.
7. Technical Guide for Smart Electric Equipments, State Grid Company Standard, Q/GDW Z 410-2010.
8. Technical Specification of Protection for Smart Substation, State Grid Company Standard, Q/GDW 441- 2010.
9. The Technical Specification for Electronic Current Transformers, State Grid Company Standard, Q/GDW 424-2010.
10. Supplementary Regulations for New Substation Design in 2011, State Grid Company, [2011] 58.
11. Suggestion of Optimally Integrated design and construction for Smart Substation, State Grid Company, [2011] 539.
12. Technical Guide for Online Monitoring System of Substation Equipments, State Grid Company Standard, Q/GDW 534- 2010.

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RESEARCH ARTICLE

The Continuous Fractional Bessel Wavelet Transformation B_{ψ}^{θ} on Some Spaces of Type H_{μ}

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ABSTRACT

The aim of the present paper is to study the "fractional Hankel transformation" (FrHT) and the "continuous fractional Bessel wavelet transformation" (CFrBWT) on some H_{μ} type spaces. The continuity of the CFrBWT on some H_{μ} type spaces is shown.

Keywords: Bessel wavelet transformation, functions, parameter

INTRODUCTION

The continuous and discrete Bessel wavelet transforms are introduced by Pathak and Dixit [9] and investigated their properties by exploiting Hankel convolution of Haimo [2] and Hirschman [3]. Prasad et al. [13] investigated the "continuous fractional Bessel wavelet transformation" and studied some of their basic properties. Upadhyay et al. [14] introduced the continuous Bessel wavelet transformation associated with the Hankel-Hausdorff operator. In a recent article, motivated by the work of Prasad et al. [13], and develop a theory of the "continuous fractional Bessel wavelet transformation" on space of type H_{μ} corresponding to [10] and [11]. We now set the following fractional differential operators which are very useful in our present study

$N_{\mu,x,\theta}\,\phi(x) = e^{\frac{i}{2}x^2\cot\theta}\, x^{\mu+1/2} D_x\, x^{-\mu-1/2} e^{-\frac{i}{2}x^2\cot\theta}\,\phi(x)$, where $D_x = \frac{d}{dx}$,

$$M_{\mu,x,\theta}\,\phi(x) = e^{\frac{i}{2}x^2\cot\theta}\, x^{-\mu-1/2} D_x\, x^{\mu+1/2}\, e^{-\frac{i}{2}x^2\cot\theta}\,\phi(x),$$

$$S_{\mu,x,\theta} = M_{\mu,x,\theta}\, N_{\mu,x,\theta} = \frac{d^2}{dx^2} - 2ix\cot\theta\frac{d}{dx} + \left(\frac{1-4\mu^2}{4x^2}\right) - i\cot\theta - x^2\cot^2\theta.$$

Also, the identity

$$S^q{}_{\mu,x,\theta}\,\phi(x) = \sum_{j=0}^{q} b_j\, e^{\frac{i}{2}x^2\cot\theta}\, x^{\mu+2j+1/2}\left(x^{-1}D\right)^{q+j}\left(x^{-\mu-1/2}\, e^{-\frac{i}{2}x^2\cot\theta}\right)\phi(x),\ \ q\in\square_0,$$

where the constant b_j depend only on $\mu \geq -\frac{1}{2}$ and θ being the parameter.

The space $L^p(\square)$ denotes the space, which consist of all real valued measurable functions ϕ on $\square$ such that the integral $\int_{\square_+} |\phi(x)|^p\, dx, \square_+ = (0,\infty)$ exist and finite. Also, let $L^\infty(\square)$ be a collection of almost everywhere bounded functions. Hence endowed with the norm

$$\square\phi\square_{L^p} = \begin{cases} \left(\int_0^\infty |\phi(x)|^p\, dx\right)^{\frac{1}{p}}, & \text{for } 1 \leq p < \infty. \\ ess\,Sup_{x\in\square}\ |\phi(x)|, & \text{for } p = \infty \end{cases}$$

The "Hankel transformation" h_μ of a conventional function $\phi \in L^1(\square_+), \square_+ = (0,\infty)$ is usually defined by Zemanian [15, p.127, equs.(1) and (2)]:

$$\hat{\phi}(x) = \left(h_\mu\phi\right)(x) = \int_0^\infty (xy)^{\frac{1}{2}} J_\mu(xy)\,\phi(y)\,dy, \quad \mu \geq -\frac{1}{2} \tag{1}$$

and its inversion formula is $\phi(y) = \left(h_\mu^{-1}\hat{\phi}\right)(y) = \int_0^\infty (xy)^{\frac{1}{2}} J_\mu(xy)\,\hat{\phi}(x)\,dx,$ (2)

where J_μ denote the first kind of Bessel function having order μ.

The "fractional Hankel transformation" is a generalization of the conventional "Hankel transformation" which depends on $\mu \geq -\frac{1}{2}$ and the angle θ, has many applications in several areas like optics, signal processing, seismology etc. Various forms of fractional Hankel transformations have been considered in [4, 6, 13, 16] as:

$$\hat{\phi}_\mu^\theta(y) = \left(h_\mu^\theta\right)(y) = \int_0^\infty K_\mu^\theta(x,y)\,\phi(x)\,dx, \tag{3}$$

where the kernel

$$K_\mu^\theta(x,y)=\begin{cases} c_\mu^\theta e^{\frac{i}{2}(x^2+y^2)\cot\theta}(xy\cos ec\theta)^{\frac{i}{2}}J_\mu(xy\cos ec\theta), & \theta\neq n\pi,\\ (xy)^{\frac{i}{2}}J_\mu(xy), & \theta=\frac{\pi}{2},\\ \delta(x-y), & \theta=n\pi,\ \forall n\in\mathbb{Z}, \end{cases}$$

where $c_\mu^\theta=\dfrac{\exp\left[i(1+\mu)\left(\frac{\pi}{2}-\theta\right)\right]}{\sin\theta}$.

The inversion formula of (3) is given by

$$\phi(x)=\left(\left(h_\mu^\theta\right)^{-1}\hat{\phi}\right)(x)=\int_0^\infty \overline{K_\mu^\theta(x,y)}\left(h_\mu^\theta\phi\right)(y)\,dy, \tag{4}$$

where $\overline{K_\mu^\theta(x,y)}=\exp\left[-i(1+\mu)(\pi/2-\theta)\right]e^{-\frac{i}{2}(x^2+y^2)\cot\theta}(xy\cos ec\theta)^{\frac{1}{2}}J_\mu(xy\cos ec\theta)$

$$=\overline{\left(c_\mu^\theta\right)}\sin\theta\, e^{-\frac{i}{2}(x^2+y^2)\cot\theta}(xy\cos ec\theta)^{\frac{1}{2}}J_\mu(xy\cos ec\theta),$$

and $\mathrm{h}_\mu^\theta\phi=\mathrm{h}_\mu^\pi\phi=\phi;\ \ \mathrm{h}_\mu^{\theta+2\pi}\phi=\mathrm{h}_\mu^\theta\phi,\ \ \forall\theta\in\mathbb{Z}$.

We assume that throughout this paper $\theta\neq n\pi, n\in\mathbb{Z}$.

Proposition 1.1. *Let us consider the kernel $K_\mu^\theta(x,y)$ of the "fractional Hankel transformation". Then*

$$\Delta_{\mu,x,\theta}^r K_\mu^\theta(x,y)=S_{\mu,x,\theta}^r K_\mu^\theta(x,y)=\left(-y^2\cos ec^2\theta\right)^r K_\mu^\theta(x,y),\qquad \forall r\in\mathbb{Z}_0,$$

where $\Delta_{\mu,x,\theta}=S_{\mu,x,\theta}=\dfrac{d^2}{dx^2}-2ix\cot\theta\dfrac{d}{dx}+\left(\dfrac{1-4\mu^2}{4x^2}\right)-i\cot\theta-x^2\cot^2\theta$ *which is known as the operator of fractional Bessel's having parameter* θ.

Proof: See [12].

From [13], A "fractional Bessel wavelet" is a function $\psi\in L^2(0,\infty)$ which satisfies the admissibility condition

$$C_{\mu,\psi,\theta}=\int_0^\infty x^{-2\mu-2}\left|\left(h_\mu^\theta\psi\right)(x)\right|^2dx<\infty,\ \ \mu\geq-\frac{1}{2}, \tag{5}$$

where $\left(h_\mu^\theta\psi\right)$ is the fractional Hankel transformation of ψ. The fractional Bessel wavelets $\psi_{b,a}^\theta$ are generated from one single function $\psi\in L^2(0,\infty)$ by dilation and translation with parameters $a>0$ and $b\geq0$ respectively, which is given by

$$\psi_{b,a}^{\theta}=\frac{1}{\sqrt{a}}\,e^{-\frac{i}{2}\left(\frac{b^2}{a^2}+\frac{x^2}{a^2}\right)\cot\theta}\int_0^{\infty}\psi(z)D_{\mu}^{\theta}\left(\frac{b}{a},\frac{x}{a},z\right)dz.$$

Lemma 1.1. *If* $\phi,\psi\in L^2(0,\infty)$. *Then the "continuous fractional Bessel wavelet transformation"* B_{ψ}^{θ} *is defined on* ϕ *by*

$$\left(B_{\psi}^{\theta}\phi\right)(b,a)=\left(\frac{\sin\theta}{a^{\mu}}\right)\overline{c_{\mu}^{\theta}}\int_0^{\infty}e^{i/2(a^2-1)x^2\cot\theta}\,x^{-\mu-1/2}\left(bx\,\mathrm{cosec}\,\theta\right)^{\frac{1}{2}}J_{\mu}\left(bx\,\mathrm{cosec}\,\theta\right)\Phi(x)\overline{\Psi}(ax)dx, \qquad (6)$$

where $\Phi=h_{\mu}^{\theta}\left[e^{-\frac{i}{2}(.)^2\cot\theta}\,\phi\right]$ *and* $\overline{\Psi}=\overline{\left(h_{\mu}^{\theta}\psi\right)}$.

Proof: See [13]

2. THE SPACES $H_{\mu,M,\alpha}$ AND $H_{\mu}^{\Omega,\beta}$.

Let $\mu(\xi),(0\le\xi<\infty)$ and $\omega(\eta),(0\le\eta<\infty)$ be continuous non-decreasing functions such that $\mu(0)=0,\ \mu(\xi)\to\infty$ for $\xi\to\infty$ and $\omega(0)=0,\omega(\eta)\to\infty$ for $\eta\to\infty$.

For $x\ge0,y\ge0,$ we define

$$M(x)=\int_0^{x}\mu(\xi)d\xi,\qquad M(x)=M(-x)\ \text{ for } x<0\,, \qquad (7)$$

and $$\Omega(y)=\int_0^{y}\omega(\eta)d\eta,\qquad \Omega(y)=\Omega(-y)\ \text{ for } y<0\,. \qquad (8)$$

The functions $M(x)$ and $\Omega(y)$ are continuous, non-decreasing and convex with $M(0)=0,\ M(x)\to\infty$ for $x\to\infty$ and $\Omega(0)=0,\ \Omega(y)\to\infty$ for $y\to\infty$. We have the following fundamental convex inequalities,

$$M(x_1)+M(x_2)\le M(x_1+x_2),\qquad \Omega(y_1)+\Omega(y_2)\le\Omega(y_1+y_2)\,. \qquad (9)$$

If the functions $\mu(\xi)$ and $\omega(\eta)$ are mutually inverse, that is, $\mu(\omega(\eta))=\eta,\ \omega(\mu(\xi))=\xi$ then the corresponding functions $M(x)$ and $\Omega(y)$ will be said to be dual in the Young sense. In this situation, the Young's inequality

$$xy\le M(x)+\Omega(y), \qquad (10)$$

holds for $x\ge0,y\ge0$.

From Gel'fand and Shilov [1], Lee [5] and Pathak and Sahoo [7], we studied the some spaces of type H_{μ}, that is, $H_{\mu,M,\alpha}$ and $H_{\mu}^{\Omega,\beta}$ are defined as follows:

Definition 2.1 The space $H_{\mu,M,\alpha}$ consists of all complex valued infinitely differentiable functions $\phi(x), (-\infty < x < \infty)$ which for any $\delta > 0$ satisfy the inequality

$$\left| S^q_{\mu,x,\theta}\left(x^{-\mu-1/2}\,\phi(x)\right)\right| \le C_{q,\delta}\exp[-M((\alpha-\delta)x)], \quad q = 0,1,2... \tag{11}$$

where $C_{q,\delta} > 0$ and α>0 *are constants which may depend on the function* ϕ .

***Definition* 2.2.** *The space* $H_\mu^{\Omega,\beta}$ *consists of all entire analytic functions* $\psi(z), (z = x + iy \in \square)$ *which for any* $\rho > 0$ *satisfy the inequality*

$$\left| z^{2k-\mu-1/2}\,\psi(z)\right| \le C_{k,\rho}\exp[\Omega((\beta+\rho)y)], \quad k = 0,1,2... \tag{12}$$

where $C_{k,\rho} > 0$ and β>0 *are constants which may depend on the function* ψ .

Theorem 2.1. *Let M(x) be the function which is dual in the sense of Young to* $\Omega(y)$ *.The functional Hankel transformation is defined by (3) with* $e^{-iz^2\cot\theta/2}\phi(z) \in H_\mu^{\Omega,\beta}(£)$. *Then the functional Hankel operator* $h_\mu^\theta : H_\mu^{\Omega,\beta}(£) \to H_{\mu,M,1/\beta}(¡)$ *is continuous and* $H_\mu^{\Omega,\beta} \subset H_{\mu,M,1/\beta}$.

Proof: Let $q \in N_0, z = x + iy$ and θ being the parameter, using the technique of [1, pp. 21-22], we have

$$\Phi(\omega) = h_\mu^\theta\left[e^{-\frac{1}{2}(z)^2\cot\theta}\phi(z)\right](\omega) = c_\mu^\theta\int_0^\infty c^{\frac{i}{2}\left(z^2+\omega^2\right)\cot\theta}\left(z\omega cse\theta\right)^{\frac{1}{2}} J_\mu\left(z\omega\csc\theta\right)e^{-\frac{i}{2}z^2\cot\theta}\phi(z)dx$$

$$S^q_{\mu,\omega,\theta}\left(\omega^{-\mu-1/2}\Phi(\omega)\right)$$
$$= S^q_{\mu,\omega,\theta}\left[\omega^{-\mu-1/2}c_\mu^\theta\int_0^\infty e^{\frac{i}{2}\left(z^2+\omega^2\right)\cot\theta}\left(z\omega cse\theta\right)^{\frac{1}{2}} J_\mu\left(z\omega\csc\theta\right)\times e^{-\frac{i}{2}z^2\cot\theta}\phi(z)dx\right]$$

Now, using the identity

$$S^q_{\mu,\omega,\theta} = \sum_{j=0}^{q} b_j e^{\frac{i}{2}\omega^2\cot\theta}\omega^{\mu+2j+\frac{1}{2}}\left(\omega^{-1}\frac{d}{d\omega}\right)^{q+j}\omega^{-\mu-1/2}$$
$$\times\int_0^\infty\left(z\omega\csc\theta\right)^{\frac{1}{2}} J_\mu\left(z\omega\csc\theta\right)\phi(z)dx$$
$$= \exp\left[i\left(1+\mu\right)\left(\frac{\pi}{2}-\theta\right)\right]\sum_{j=0}^{q} b_j e^{\frac{i}{2}\omega^2\cot\theta}\left(z\omega\right)^{2j}\frac{1}{\left(\sin\theta\right)^{\mu+3/2+2(q+j)}}$$
$$\times(-1)^{q+j}\int_0^\infty\left(z\omega\csc\theta\right)^{-(\mu+q+j)} J_{\mu+q+j}\left(z\omega\csc\theta\right)z^{(\mu+2q+1/2)}\phi(z)dx.$$

$$\text{Therefore, } \left|S^{q}_{\mu,\omega,\theta}\left(\omega^{-\mu-1/2}\Phi(\omega)\right)\right| \le \sum_{j=0}^{q}\left|b_j\right|\left|e^{2j\log(z\omega)}\right|\frac{1}{\left|\sin\theta\right|^{(mu+3/2+2(q+j))}}$$
$$\times\int_0^{\infty}\left|\left(z\omega\csc\theta\right)^{-(\mu+q+j)}J_{\mu+q+j}\left(z\omega\csc\theta\right)\right|\left|z^{(\mu+2q+1/2)}\phi(z)\right|dx.$$

As in [8, p. 247], and $\log(z\omega)\le z\omega$ for $z>0$ and $\omega>0$, we can estimate the above expression as follows:

$$\left|S^{q}_{\mu,\omega,\theta}\left(\omega^{-\mu-1/2}\Phi(\omega)\right)\right| \le \sum_{j=0}^{q}\left|b_j\right|\left|e^{2j(z\omega)}\right|\frac{1}{\left|\sin\theta\right|^{(mu+3/2+2(q+j))}}$$
$$\times C_{\mu,\theta}\int_0^{\infty}\left|z^{(\mu+2q+1/2)}\phi(z)\right|dx$$
$$\le C'_{\mu,\sin\theta}\sum_{j=0}^{q}\left|b_j\right|\left|e^{2jz\omega}\right|\int_0^{\infty}\left|z^{(\mu+2q+1/2}\phi(z)\right|dx.$$

Now, using the inequality $\left|z\right|^{l}\le\dfrac{\left|z\right|^{l+2}+\left|z\right|^{l}}{\left(x^2+1\right)}$, we have

$$\left|S^{q}_{\mu,\omega,\theta}\left(\omega^{-\mu-1/2}\Phi(\omega)\right)\right| \le C'_{\mu,\sin\theta}\sum_{j=0}^{q}\left|b_j\right|\left|e^{2jz\omega}\right|\left[\left(\left|z\right|^{\mu+2q+5/2}+\left|z\right|^{(\mu+2q+1/2)}\right)\phi(z)\right]\times\int_0^{\infty}\frac{dx}{x^2+1}$$

$$\le C'_{\mu.\sin\theta}e^{|2qz\omega|}\sum_{j=0}^{q}\left|b_j\right|\left|\left[\left(1+z^2\right)^{\mu+q+3/2}+\left(1+z^2\right)^{\mu+q+1/2}\right]z^{(-\mu-1/2)}\phi(z)\right|.$$

Let ξ be the positive integers, such that $\xi\ge q+\mu+1/2\ge 0.$ Then we obtain the estimate

$$\left|S^{q}_{\mu,\omega,\theta}\left(\omega^{-\mu-1/2}\Phi(\omega)\right)\right| \le C'_{\mu.\sin\theta}e^{|-2qy\omega|}\sum_{j=0}^{q}\left|b_j\right|$$
$$\times\left|\left[\sum_{u=0}^{\xi+1}\binom{\xi+1}{u}z^{2u-\mu-1/2}\phi(z)+\sum_{v=0}^{\xi}\binom{\xi}{v}z^{2v-\mu-1/2}\phi(z)\right]\right|.$$

Now, using the Definition 2.2, the last expression can be estimated by

$$C'_{\mu,\sin\theta}e^{|-2q\omega y|}\sum_{j=0}^{q}\left|b_j\right|\left[\sum_{u=0}^{\xi+1}\binom{\xi+1}{u}C_{u,\rho}\exp\left[\Omega\left((\beta+\rho)y\right)\right]\right]$$
$$+\left[\sum_{v=0}^{\xi}\binom{\xi}{v}C_{u,\rho'}\exp\left[\Omega((\beta+\rho')y)\right]\right]$$

$$\leq C'_{\mu,\sin\theta}\sum_{j=0}^{q}\left|b_j\right|\left(\sum_{u=0}^{\xi+1}\binom{\xi+1}{u}C_{u,\rho}+\sum_{v=0}^{\xi}\binom{\xi}{v}C_{u,\rho}\right)$$

$$\times\exp\left[\Omega((\beta+\rho)y-2q\omega y\right] \text{ for } \rho'=\rho$$

$$\leq C^{u}_{\xi,\rho,\sin\theta}\sum_{j=0}^{q}\left|b_j\right|\exp\left[\Omega((\beta+\rho)y)-2q\omega y\right]. \tag{13}$$

Let us now choose the sign of y in such a way that the equality $2q\omega y=2q\left|\omega\right|\left|y\right|$ be satisfied and the absolute value of y, so that the inequality of Young's with $|y|$ replaced by $(\beta+\rho)|y|$ and ω replaced by $\frac{|\omega|}{2q(\beta+\rho)}$ yields the equality

$$2q\left|\omega\right|\left|y\right|=M\left(\frac{\left|\omega\right|}{(\beta+\rho)}\right)+\Omega\left((\beta+\rho)\left|y\right|\right).$$

Then the exponent in (13) yields

$$\Omega\left((\beta+\rho)y\right)=2q\omega y=-M\left(\frac{\left|\omega\right|}{(\beta+\rho)}\right)$$

Hence, $\left|S^{q}_{\mu,\omega,\theta}\left(\omega^{-\mu-1/2}\,\Phi(\omega)\right)\right|\leq C^{u}_{\xi,\rho,\sin\theta}\sum_{j=0}^{q}\left|b_j\right|\exp\left[-M\left(\frac{\left|\omega\right|}{(\beta+\rho)}\right)\right].$

In the above expression, we set $\frac{1}{(\beta+\rho)}=\frac{1}{\beta}-\delta,$ where δ arbitrary small is; we obtain the above expression which can be bounded by

$$\left|S^{q}_{\mu,\omega,\theta}\left(\omega^{-\mu-1/2}\,\Phi(\omega)\right)\right|\leq C^{m}_{q,\xi,\delta,\sin\theta}\exp\left[-M\left(\left(\frac{1}{\beta}-\delta\right)\omega\right)\right].$$

Theorem 2.2. *Let M(x) and* $\Omega(y)$ *be a pair of functions which are dual in Young sense. The fractional Hankel transformation which is given in (3) with* $e^{-ix^2\cos t\theta/2}\phi(x)\in H_{\mu,M,\alpha}(¡\ )$. *Then the operator of fractional Hankel* $h^{\theta}_{\mu}:H_{\mu,M,\alpha}(¡\ )\to H^{\Omega,1/\alpha}_{\mu}(£\ )$ *is continuous and* $H^{\%}_{\mu,M,\alpha}\subset H^{\Omega,(1/\alpha+\varepsilon)}_{\mu}$ *for* $\alpha,\varepsilon>0.$ *That is the fractional Hankel-dual of* $H_{\mu,M,\alpha}$ *is included in* $H^{\Omega,(1/\alpha+\varepsilon)}_{\mu}$ *space.*

Proof: Let $\sigma = \omega + i\tau$ and θ being the parameter, using the technique of [1, pp. 20-21], we have

$$\begin{aligned}\Phi(\omega) &= h_\mu^\theta\left[e^{-\frac{i}{2}(x)^2\cot\theta}\phi(x)\right](\omega)\\ &= c_\mu^\theta\int_0^\infty e^{\frac{i}{2}\left(x^2+\omega^2\right)\cot\theta}\left(x\omega\csc\theta\right)^{1/2}J_\mu\left(x\omega\csc\theta\right)e^{-\frac{1}{2}x^2\cot\theta}\phi(x)dx.\end{aligned}$$

$$\begin{aligned}(-1)^q\left(\omega\csc\theta\right)^2\Phi(\omega) &= \int_0^\infty(-1)^q c_\mu^\theta\left(\omega\csc\theta\right)^{2q}e^{\frac{1}{2}\left(x^2+\omega^2\right)\cot\theta}\\ &\quad\times\left(\omega\csc\theta\right)^{\frac{1}{2}}J_\mu\left(x\omega\csc\theta\right)e^{-\frac{i}{2}x^2\cot\theta}\phi(x)dx.\end{aligned}$$

Now using the Proposition 1.1, the above expression can be estimated by

$$\frac{(-1)^q}{\left(\sin\theta\right)^{2q}}\omega^{2q}\Phi(\omega) = c_\mu^\theta e^{\frac{i}{2}\omega^2\cot\theta}\int_0^\infty S_{\mu,x,\theta}^q\left[\phi(x)\right](x\omega\csc\theta)^{\frac{1}{2}}J_\mu\left(x\omega\csc\theta\right)dx.$$

Therefore,

$$\begin{aligned}&\frac{(-1)^q}{\left(\sin\theta\right)^{2q-\mu-1/2}}\left(\omega+i\tau\right)^{2q-\mu-1/2}\Phi(\omega+i\tau) = c_\mu^\theta e^{\frac{i}{2}(\omega+i\tau)^2\cot\theta}\int_0^\infty S_{\mu,x,6\theta}^q\left[\phi(x)\right]x^{-\mu-1/2}\\ &\times\ x^{2\mu+1}\left(x(\omega+i\tau)\csc\theta\right)^{-\mu}J_\mu\left(x(\omega+i\tau)\csc\theta\right)dx\\ &(-1)^q\sigma^{2q-\mu-1/2}\Phi(\sigma) = \exp\left[i(1+\mu)(\pi/2-\theta\right](\sin\theta)^{2q-\mu-3/2}e^{\frac{i}{2}(\omega^2-\tau^2)\cot\theta}\\ &\times e^{-\omega\tau\cot\theta}\int_0^\infty S_{\mu,x,\theta}^q\left[\phi(x)\right]x^{-\mu-1/2}e^{(2\mu+1)\log x}(x\sigma\csc\theta)^{-\mu}J_\mu(x\sigma\csc\theta)dx.\end{aligned}$$

Therefore,

$$\begin{aligned}\left|\sigma^{2q-\mu-1/2}\Phi(\sigma)\right| &\le \left|\sin\theta\right|^{(2q-\mu-3/2)}\int_0^\infty\left|(x\sigma\csc\theta)^{-\mu}J_\mu(x\sigma\csc\theta)e^{-\omega\tau\cot\theta}\right|\\ &\quad\times\left|e^{(2\mu+1)\log x}\right|\left|S_{\mu,x,\theta}^q x^{-\mu-1/2}\phi(x)\right|dx.\end{aligned}$$

Since $\phi\in H_{\mu,M,\alpha}$, $\log x < x$ and from [8, p. 310], the last expression can be estimated by

$$\left|\sigma^{2q-\mu-1/2}\Phi(\sigma)\right| \le C'_{q,\delta,\sin\theta}e^{-\mu|\tau|}\int_0^\infty\exp\left[-M((\alpha-\delta)x)+(2\mu+1+|\tau|)x\right]dx. \tag{14}$$

Using the Young's inequality (10), we have

$$\left(2\mu+1+|\tau|\right)x = \gamma x\left(\frac{1}{\gamma}(2\mu+1+|\tau|\right) \le M\left(\gamma x\right)+\Omega\left[\frac{1}{\gamma}(2\mu+1+|\tau|)\right],\ \text{with}\ \gamma=(\alpha-2\delta).$$

Then, the exponent in (14) is less than or equal to $-M\left[(\alpha-\delta)x\right]+M(\gamma x)+\Omega\left[\frac{1}{\gamma}(2\mu+1+|\tau|\right].$

Thus, we derive the estimate

$$\left|\sigma^{2q-\mu-1/2}\Phi(\sigma)\right| \le C'_{q,\delta,\sin\theta} e^{\omega|\tau|} e^{\Omega\left[\frac{1}{\gamma}(2\mu+1+|\tau|\right]} \int_0^\infty e^{-M|\delta x|} dx. \qquad (15)$$

From Gelfand and Shilov [1, p. 18] and Pathak and Sahoo [7, p.138], we obtain

$e^{\omega|\tau|} \le e^{\Omega(\varepsilon\tau)} + C_1$ and $e^{\Omega\left[\frac{1}{\gamma}+(2\mu+1+|\tau|)\right]} \le e^{\left(C_\mu+\Omega[(2\mu+1+1/\gamma]|\tau|\right)} \le e^{(C_\mu+\Omega[|(1/\alpha+\rho)\tau|]}$, where $\rho > 0$.

Hence $\left|\sigma^{2q-\mu-1/2}\Phi(\sigma)\right| \le C''_{q,\rho,\sin\theta} \exp^{[\Omega((1/\alpha+\rho+\varepsilon)\tau)]}$.

Due to fact that the right-hand side of the integral of (15) is bounded by $\int_0^\infty e^{-M|\delta x|} dx < \infty$.

Therefore, $H^{0}_{\mu,M,\alpha} \subset H_\mu^{\Omega(1/\alpha+\varepsilon)}$ for $\alpha, \varepsilon > 0$.

We modified the definition of Pathak and Pandey [10] and Prasad and Mahato [11] for the following similar test function space, known as H_μ - type space which will be applied in the study of the "continuous fractional Bessel wavelet transformation".

Definition 2.3. The space $H_\mu^{*,\Omega,\Omega,\alpha,a\alpha}$, where $\alpha > 0$, is defined to be the set of all entire analytic functions $\phi_a(\zeta) = \phi(\zeta, a) \in C^\infty(\mathbb{R} \times \mathbb{R}_+)$ with respect to $\zeta = b + i\lambda$ which for any $\rho, \rho' > 0$ satisfy the inequality

$$\left|S^t_{\mu,a,\theta}\left(\frac{1}{\sqrt{a}}\phi(\zeta,a)\right)\right| \le C_{t,\rho} \exp\left[\Omega\{\lambda(a+\rho)\} + \Omega\{\lambda(a\alpha+\rho')\}\right], \quad t = 0,1,2... \qquad (16)$$

where $C_{t,\rho} > 0$ is a constant depending on the function.

THE CONTINUOUS FRACTIONAL BESSEL WAVELET TRANSFORMATION

In this section, we study the "continuous fractional Bessel wavelet transformation" defined by (6) on the spaces $H_{\mu,M,\alpha}$ and $H_\mu^{\Omega,\beta}$.

Theorem 3.1. Let $M(x)$ and $\Omega(y)$ be the functions which are dual in the sense of Young. Let $\Psi \in H_{\mu,M,\alpha}$ and $\Phi \in H_{\mu,M,\alpha}$, then the "continuous fractional Bessel wavelet transformation"

$\left(B^\theta_\psi \phi\right)(\zeta,a) \in H_\mu^{*,\Omega,\Omega,1/\alpha,1/a\alpha}$, $\zeta = b + i\lambda$, that is, the "continuous fractional Bessel wavelet transformation" $\left(B^\theta_\psi \phi\right)(\zeta,a)$ is a continuous linear map from $H_\mu^{\Omega,1/\alpha}$ into $H_\mu^{*,\Omega,\Omega,1/\alpha,1/a\alpha}$.

Proof: *The "continuous fractional Bessel wavelet transformation" of a function ϕ with respect to the wavelet ψ defined by (6) is*

$$\left(B^\theta_\psi \phi\right)(b,a) = a^{-\mu}\sin\theta\ \overline{c^\theta_\mu} \int_0^\infty e^{i/2(a^2-1)x^2\cot\theta}\, x^{-\mu-1/2} \left(bx\,\mathrm{cos}\,ec\theta\right)^{\frac{1}{2}} J_\mu\left(bx\,\mathrm{cos}\,ec\theta\right)\Phi(x)\overline{\Psi}(ax)dx.$$

Since both Φ *and* $\Psi \in H_{\mu,M,\alpha}$ *, therefore, the "continuous fractional Bessel wavelet transformation" can be extended to the complex values of* $\zeta = b + i\lambda$ *according to the definition*

$$\left(B_{\psi}^{\theta}\phi\right)(b+i\lambda,a) = a^{-\mu}\sin\theta\overline{c_{\mu}^{\theta}}\int_0^{\infty} e^{\frac{i}{2}(a^2-1)x^2\cot\theta}x^{-\mu-1/2} \times((b+i\lambda)x\csc\theta)^{\frac{i}{2}}J_{\mu}((b+i\lambda)x\csc\theta)\Phi(x)\overline{\Psi}(ax)dx.$$

$$(B_{\psi}^{\theta}\phi)(\zeta,a) = a^{-\mu}\sin\theta\overline{c_{\mu}^{\theta}}\int_0^{\infty} e^{\frac{i}{2}(a^2-1)x^2\cot\theta}x^{-\mu-1/2} \times\left(\zeta x\csc\theta\right)^{\frac{i}{2}}J_{\mu}\left(\zeta x\csc\theta\right)\Phi(x)\overline{\Psi}(ax)dx$$

$$\frac{1}{\sqrt{a}}(B_{\psi}^{\theta}\phi)(\zeta,\alpha) = a^{-\mu-1/2}\exp\left[-i\left(1+\mu\right)(\pi/2-\theta)\right]\frac{1}{(\sin\theta)^{\mu+1/2}}\int_0^{\infty} e^{\frac{i}{2}(a^2-1)x^2\cot\theta} \times e^{(\mu+1/2)\log\zeta}\left(\zeta x\csc\theta\right)^{-\mu}J_{\mu}\left(\zeta x\csc\theta\right)\Phi(x)\overline{\Psi}(ax)dx.$$

For non-negative integer t, we obtain

$$\left|S'_{\mu,a,\theta}\left[\frac{1}{\sqrt{a}}\left(B_{\psi}^{\theta}\phi\right)(\zeta,a)\right]\right| \le \frac{1}{|\sin\theta|^{\mu+1/2}}\int_0^{\infty}\left|e^{(\mu+1/2)\log\zeta}\left(\zeta x\csc\theta\right)^{-\mu}J_{\mu}\left(\zeta\csc\theta\right)\right| \times\left|\Phi(x)\right|\left|S_{\mu,a,\theta}^{t}\left(a^{-\mu-1/2}\overline{\Psi}(ax)\right)\right|dx.$$

Since $\log\zeta < \zeta$, we can derive the estimate

$$\left|S_{\mu,a,\theta}^{t}\left[\frac{1}{\sqrt{a}}\left(B_{\psi}^{\theta}\phi\right)(\zeta,a)\right]\right| \le \frac{1}{|\sin\theta|^{\mu+1/2}}\int_0^{\infty}\left|(\zeta x\csc\theta)^{-\mu}J_{\mu}(\zeta x\csc\theta)e^{(\mu+1/2)\zeta}\right| \times\left|\Phi(x)\right|\left|S_{\mu,a,\theta}^{t}\left(a^{-\mu-1/2}\overline{\Psi}(ax)\right)\right|dx.$$

As in [8, p.310], the above expression can be estimated by

$$\left|S_{\mu,a,\theta}^{t}\left[\frac{1}{\sqrt{a}}\left(B_{\psi}^{\theta}\phi\right)(\zeta,a)\right]\right| \le \frac{1}{|\sin\theta|^{\mu+1/2}}C_{\mu,\theta}\int_0^{\infty}\exp\left[x|\lambda|+(\mu+1/2|\lambda|\right] \times\left|\Phi(x)\right|\left|S_{\mu,a,\theta}^{t}\left(a^{-\mu-1/2}\overline{\Psi}(a)\right)\right|dx.$$

Now, using the definition 2.1, we obtain

$$\left|S_{\mu,a,\theta}^{t}\left[\frac{1}{\sqrt{a}}\left(B_{\psi}^{\theta}\phi\right)(\zeta,a)\right]\right| \le \frac{1}{|\sin\theta|^{\mu+1/2}}C_{\mu,\theta}\int_0^{\infty}\exp\left[(x+\mu+1/2)|\lambda|\right] \times C_{0,\delta}\exp\left[-M\left((\alpha-\delta)x\right)\right]c_{t,\delta'}\exp\left[-M\left((\alpha-\delta')ax\right)\right]dx$$

$$\le C'_{t,\delta,\delta',\sin\theta}\int_0^{\infty}\exp\left[2\left(x+\mu+1/2\right)|\lambda|-M\left((\alpha-\delta)x\right)-M\left((\alpha-\delta')ax\right)\right]dx.$$

Now, applying fundamental convex inequality (9) and the inequality of Young's (10), the exponent in the above integral can be transformed as:

$$-M\left[(\alpha-\delta)x\right]+(x+\mu+1/2)|\lambda|\le -M|\delta x|+\Omega\left[\frac{\lambda}{\alpha-2\delta}\right]$$

$$\text{and}\quad -M\left[(\alpha-\delta')x\right]+(x+\mu+1/2)|\lambda|\le -M|\delta' x|+\Omega\left[\frac{\lambda}{\alpha-2\delta'}\right]$$

Therefore, we obtain the estimate

$$\left|S^{t}_{\mu,a,\theta}\left[\frac{1}{\sqrt{a}}\left(B^{\theta}_{\psi}\phi\right)(\zeta,a)\right]\right|\le C'_{t,\delta,\delta',\sin\theta}\exp\left[\Omega\left(\frac{\lambda}{\alpha-2\delta}\right)+\Omega\left(\frac{\lambda}{a(\alpha-2\delta')}\right)\right]$$

$$\times\int_0^{\infty}e^{-M|\delta x|-M|\delta' ax|}dx,$$

Due to [1, p.21] fact that the integral $\int_0^{\infty}e^{-M|\delta x|-M|\delta' ax|}dx$ has a finite value. The quantities $\frac{1}{(\alpha-2\delta)}$ and $\frac{1}{a(\alpha-2\delta')}$ can be represented in the form $\frac{1}{\alpha}+\rho$ and $\frac{1}{a\alpha}+\rho'$ respectively, where ρ and ρ' are arbitrary small together with δ and δ' respectively. We thus obtain the above expression can be bounded by

$$C''_{t,\rho,\rho',\sin\theta}\exp\left(\Omega\left[\lambda\left(\frac{1}{\alpha}+\rho\right)\right]+\Omega\left[\lambda\left(\frac{1}{a\alpha}+\rho'\right)\right]\right).$$

Thus, $\left(B^{\theta}_{\psi}\phi\right)(\zeta,a)\in H^{0,\Omega,\Omega,1/\alpha,1/a\alpha}_{\mu}$.

REFERENCES

1. I. M. Gel'fand and G. E. Shilov, Generalized Functions, Academic Press, New York, Vol. 3, 1967.
2. D. T. Haimo, Integral equations associated with Hankel convolution, Trans. Amer. Math. Soc., Vol. 116 (1965), 330-375.
3. I. I. Hirschman Jr, Variation diminishing Hankel transform, J. Anal. Math., Vol. 8 (1960-1961), 307-336.
4. F. H. Kerr, Fractional powers of Hankel transforms in the Zemanian spaces, J. Math. Anal. Appl., Vol. 166 (1992), 65-83.
5. W. Y. K. Lee, On spaces of type H_{μ} and their Hankel transform, SIAM J. Math. Anal., Vol. 5 (1974), 336-347.
6. V. Namias', Fractionalization of Hankel transform, J. Inst. Math. Appl., Vol. 26 (1980), 187-197.
7. R. S. Pathak and H. K. Sahoo, A generalization of H_{μ} spaces and Hankel transforms, J. Anal. Math., Vol. 12 (1986), 129-142.
8. R. S. Pathak, Integral transforms of generalized functions and their applications, Gordon and Breach Science Publishers, Amsterdam, 1997.
9. R. S. Pathak and M. M. Dixit, Continuous and discrete Bessel wavelet transforms, J. Comput. Appl. Math., Vol. 160(1-2) (2003), 241-250.
10. R. S. Pathak and G. Pandey, Wavelet transform on spaces of type W, Rocky Mountain J. Math., Vol. 39(2) (2009), 619-631.
11. A. Prasad and A. Mahato, The fractional wavelet transform on spaces of type W, Integral Transforms and Spec. Funct., Vol. 24(3) (2013), 239-250.

12. A. Prasad and V. K. Singh, The fractional Hankel transform of certain tempered distributions and pseudo-differential operators, Ann. Univ. Ferrara, Vol. {59}(1) (2013), 141-158.
13. A. Prasad, A. Mahato V. K. Singh and M. M. Dixit, The continuous fractional Bessel wavelet transformation, Bound. Value Probl., Vol. 40 (2013), 1-16.
14. S. K. Upadhyay, R. N. Yadav and L. Debnath, On continuous Bessel wavelet transformation associated with the Hankel-Hausdorff operator, Integral Transforms and Spec. Funct., Vol. 23(5) (2012), 315-323.
15. A. H. Zemanian, Generalized integral transformations, Interscience Publishers, New York, (1968).
16. Y. Zhang, T. Funaba and N. Tanno, Self-fractional Hankel functions and their properties, Opt. Commun., Vol. 176 (2000), 71-75.

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REVIEW ARTICLE

Enhanced Thermal Conductivity of Nano-Fluids and Its Affecting Factors: A Literature Review

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ABSTRACT

A review study is conducted based on the available literature in Nano-fluids and their enhanced thermal conductivity. The cooling of devices generally involves the flow of a highly conductive fluid within the channels or over plane sheets of the apparatus involved. Nano-fluids are known, basically, due to their enhanced thermal conductivity. The thermal conductivity increases with the increase in the density of nano-particles in the critical range. Several parameters (size, shape, clustering, collision, porous layer, melting point of nanoparticles) affect the thermal conductivity of nano-fluids. Nano-fluids are the advanced heat transfer fluids for the present as well as next generation.

Keywords: Nano-fluids, heat transfer and thermal conductivity.

INTRODUCTION

Nano-fluid is a fluid composed of nanometer-sized particles, called nanoparticles. These fluids are colloidal suspensions of nanoparticles in the base-liquid. Nanoparticles used in nano-liquids are usually made of metals, oxide carbides, or carbon nanotubes. Water, ethylene glycol and oil are common base fluids.Nano-fluids are known for their improved thermal conductivity, basically.

SYNTHESIS OF NANO-FLUID:

Nano-fluids are generally produced using one of the following two ways:

i. One step method

ii. Two step method

In the 1st method, there is simultaneous production of nanoparticles and dispersion of the nanoparticles in a base fluid. Using this method we can't synthesize nano-fluids in large scale. Also cost of the nano-fluid produced is very high. This is the major drawback of this method.

In the 2nd method, the nanoparticles are first produced as dry-powder by various mechanical, physical and chemical pathways such as milling, grinding and sol-gel and vapor phase methods then dispersed into the host fluid with the help of ultrasonic vibrator, high shear mixing device, intensive magnetic forceagitation etc. This is the most economical way to produce nano-fluid on a large scale.

NEEDS OF NANO-FLUID

Now-a-days a great impetus could be observed for the development of sustainable sources of energy owing to the depletion of convectional energy sources. Hence there has been a rapid innovation in several domains of science and technology. Heating and cooling of electronic devices, gadgets and metallic baths in metallurgy is one such domain. The cooling of devices generally involves the flow of a highly conductive fluid within the channels or over plane sheets of the apparatus involved. Hence scientists are in a process to improve the heat transfer capacity of the fluid so that heat exchange takes place in a faster manner. Most fluids have limited capacity to heat-up and low thermal conductivity which ultimately reduces its performance in heat exchange. To overcome the problems of low conductivity, researchers are forced to develop fluids with enhanced thermal conductivities.

APPLICATIONS OF NANO-FLUID

Nano-fluids are frequently being used in heating and cooling of electronic devices, gadgets and metallic baths in metallurgy etc. Few important applications (but not limited) are as follows:

- ✓ pharmaceutical processes
- ✓ heat transfer processes
- ✓ heat exchanger
- ✓ engine cooling
- ✓ chiller
- ✓ vehicle thermal management
- ✓ domestic refrigerators
- ✓ high power microwave tube

LITERATURE SURVEY

In the present century (i.e. the age of technology invention), there is a high demand of fluids with high thermal conductivity. To overcome the problems of low conductivity, researchers are forced to develop fluids with enhanced thermal conductivities. Choi and Eastman [1] initiated research in this direction and coined the term "nano-fluid" to refer fluids with suspended nanoparticles. These fluids have peculiar and improved thermo-physical properties. Choi et al. [2] encountered that thermal conductivity of the base fluids (conventional fluids) could be enhanced (around 40% to 150%) significantly by mixing a small amount (<1% volume fraction) of nanometre-sized-particles in the base fluid. To have a clear understanding about the latest advancements in the field of nano-fluid flow, a brief literature review has been done considering the investigations during the present decade. Some important research works have been mentioned below:

Khan and Pop [3] studied "boundary-layer flow of a nano-fluid past a stretching sheet". The investigation carried out to describe the development of boundary layer flow in steady conditions. They considered Brownian motion and thermophoresis effects in their problem. They found that theNusselt number was a decreasing function and that the Shrewood number was an increasing function of the Brownian diffusion, thermophoretic diffusion, Prandtl number, Lewis number. Ho *et al* [4]. Performed a study on "an investigation of forced convective cooling performance of a microchannel heat with Al_2O_3/water nanofluid". Here the experimental results are discussed regarding the performances of a copper microchannel heat sink cooled by alumina-water nano-fluid of 1 and 2 volume %. It is observed that for the maximal flow rate for the nano-fluid of 1 volume %.They noticed that there is an increment in the coefficient of average heat transfer by 70% compared with that of water. At the same time, the thermal resistance and the maximum wall temperature of the heat sink can be reduced by 25%. The results obtained from the

experiment are far beyond the concept of distances and variations of materials such as nanoparticle volume fraction, geometry of heat transfer etc. Hamad [5] examined "an analytical solution for the natural flow of nano-fluid flow over a high-pressure space where magnetic fields are high". It can be seen that the magnitude of the boundary layer thickness decreases, with the increase in the statistical curve, and when the magnitude of the thermal boundary layer increases. When the nanoparticle volume fraction increases, the heat transfer rates decrease. For a given value of ϕ, the heat transfer rates decrease with the increase of the value of M. The skin friction increases when M increases for a given value of f and when M is very small, the skin friction increases as ϕ increases, whereas for large values of M the skin friction decreases when ϕ increases.

Hady et al [6] studied "Radiation effect on viscous flow of a nano-fluidand heat transfer over a nonlinearly stretchingsheet". They have extended the work of Cortell [7] by considering steady thermal boundary-layer flow through nonlinear stretching surface in a nano-fluid. It was observed that, skin friction increases with increase in solid volume fraction (ϕ) and non-linear stretching parameter (n). Stretching parameter (n) and radiation parameter (N_R) are the cause for the increment in rate of heat transfer. TiO_2 nanoparticles found to have highest cooling performance in comparison to other nanoparticles (Cu and Al_2O_3).

Motsumi and Makinde [8] studied "Effects of thermal radiation and viscous dissipation on boundary layer flow of nanofluids over a permeable moving flat plate". They analyzed the problem of boundary layer nano-fluid flow through a moving permeable flat surfaceconsidering the effects ofthermal radiation, viscous dissipation and wall suction into account. Following are their findings:

- "Alumina exhibits a velocity boundary thicker than water-Cu nano-fluid. The magnitude of the velocity boundary decreases with the increase in the suction at the plate".
- "Alumina exhibits a thermal boundary layer more than Cu nano-fluid. The thickness of the thermal boundary layer increases with increasing values of r, ϕ, Br, and decreases by increasing the values of N, f_w ".
- "Skin-friction increases with increase in volumefraction ϕ; water-Cu nano-fluid exhibits higher skin-friction than alumina ".
- "The heat transfer rate at the plate surface decreases with increasing the amount of Brinkmann (Br), radiation(N) and velocity ratio parameter (r), and it increases with the suction rate f_w and nanoparticle solidfraction (ϕ)".

Singh et al [9] studied experimentally and numerically the hydrodynamics of nano-fluids in microchannels. Three microchannels of hydraulic diameters of 130, 211 and 300 lm were made using a photolithographic and aqueous system using silicon wafers. Alumina nano-fluid with concentrations of 0.25 vol %, 0.5 vol% and 1.0 vol% with particle sizes of 45 nm and 150 nm. The friction behavior of nano-fluids in microchannel is the main objective of the study. It can be seen that the cross linking properties of nano-fluids in the microchannel depend on the channel size, particle interaction and material appearance and are evident in the turbulent regime. Kalteh et al [10] carried out a research on"Experimental and numerical investigation of nano-fluid flow and heat transfer inside a microchannel heat exchangers". It was conducted both experimentally and numerically. Microchannel made of silicon wafer with glass layers used in experimental studies and the two-phase Eulerian-method utilizing a finite-volume method adopted in the numerical study. Uddin et al [11] investigated "Scaling Group Transformation for MHD Boundary Layer Slip Flow of Nanofluid over a Stretching Sheet with Heat Generation". The work being done is emphasized in the MHD movement in presence of heat generation/absorption. It is found that for the hydrodynamic boundary layer there is no -slip boundary conditions.

Makinde et al [12] investigated "Buoyancy effects on MHD stagnation point flow and heat transfer of a nanofluid past a convectively heated stretching/shrinking sheet". Here the combined effects of buoyancy force and convective heating are discussed. It is observed that the maximum speed increases with the simple velocity. Declines in temperature with increasing effects of magnetic and buoyancy. Skin friction decreases with the increase in Prandtl number. Akbar et al [13] studied "Radiation effects on MHD stagnation point flow of nanofluid towards a stretching surface with convective boundary condition". They performed their study by taking into account the consequences of radiation and convective boundary conditions.Velocity $f'(\eta)$ is found to decrease with the increase of the magnetic parameter (M) and temperature $\theta(\eta)$ and nanoparticle fraction $\phi(\eta)$ increase with increase in the value of M .The rate of heat transfer and the coefficient of skin friction decreased with the increase in Nb , Nt and $\Pr$.

Khan and Pop [14] investigated "Boundary Layer Flow Past a Wedge Moving in a Nanofluid". At the stretching surface temperature and nanoparticle fraction was taken constant. It is observed that the velocity upward increased or decreased with stretching/shrinking of the sheet. Both thermophoresis and Brownian diffusion are the cause for an increment in temperature. Das et al [15] investigated "numerical simulation of nanofluid flow in the form of convective parameters". The model incorporates Brownian flow and thermophoresis in the presence of thermal radiation, chemical reactions and magnetic fields. Governing equations are solved using Lie group transformations. The thermal boundary layer increases with the increase of the convection parameter, the thermal radiation parameter, the Brownian mobility parameter and the thermophoretic parameter. Nanofluid accumulation is a growing function of thermophoresis and convection. The mass transfer rate in the wall decreases with an increase in the convection parameter and thermophoreticparameter.

Hasan et al [16] investigated MHD radiative heat and mass transfer flow of nano-fluid in a rotating device, through a horizontal stretching wall. Radiative heat and mass transfer flowing through a horizontal stretch sheet in a rotating device was explored in detail in the presence of a strong magnetic field. Result shows that temperature increases with increase in the Brownian and Thermophoresis parameter but concentration decreases for increasing the Brownian parameter. As the Radiation parameter increases then the temperature gradually increases and the concentration decreases. Krishnamurthy et al [17] investigated effect of chemical reaction of Williamson nanofluid in porous medium on the MHD boundary layer flow with melting heat transfer. The main emphasis in the research is to discuss the nanoparticles analysis of the Williamson fluid model. It is observed that the temperature profile increases with increasing values of Nt , Nb , and the Prandtl number. The increase in skin elasticity and the Nusselt number of localized Williamson fluid nanoparticles is larger than the absence. The local Nusselt number is rising with the increase in Nb and Nt on the melting and non-melting surfaces. With Nb and Nt , in the case of melting surfaces, the heat transfer shows very little improvement.

Makinde and Animasaun [18] investigated Bioconvection in MHD nano-fluid flow with nonlinear radiation and chemical quartic autocatalysis reaction through a pioneering paraboloid's upper surface. Quartic autocatalysis of a homogeneous-heterogeneous chemical reaction was explored in this model, where the catalyst concentration on the surface is more significant. Local skin friction is optimum for thickness parameter and magnetic parameter at smaller values. For larger values of the Prandtl number and smaller temperature values, local heat transfer rate is maximum. Pandey and Kumar [19] studied "Effect of viscous dissipation and suction/injection on MHD nanofluid flow over a wedge with porous medium and slip". Results obtained in the investigation show that, with an increase in the value of Eckert number, porosity parameter and slip parameter the velocity profiles of Cu -water nano-fluid increase. The nanoparticle temperature decreases with an increase in the suction parameter as it works contrary to the injection parameter. The coefficient of skin friction increases with an increase in the Eckert number. The heat transfer rate increases with the slip parameter values increasing.

Kishan et al [20] investigated "MHD Boundary Layer Flow of a Nanofluid over an Exponentially Permeable Stretching Sheet with radiation and heat Source/Sink". The main aim of the study is to predict effects of Brownian motion, thermophoresis, and radiation on the heat and mass distribution along the nano-fluid flow boundaries. The findings obtained show that the velocity, temperature and volume fraction of the nanoparticles decrease with the increase of the magnetic field. The fraction of the volume of nanoparticles decreases with an increase of the number of Prandtl and Lewis, and the temperature decreases with the amount of Prandtl & Lewis numbers. Radiation parameter improves speed, temperature and reduces the volume fraction of nanoparticles. Sandeep and Kumar [21] examined the flow of nano-fluid through astretchable inclined wallwith a nanoparticles and dust fraction of volume considering heat and mass transfer. Here Cu -water nanofluid was embedded with conducting dust particles. It is found that, by increasing the volume fraction of nano particles, heat and mass transfer, thermal transport of the dusty nanofluid is improved. The chemical reaction parameter slows down the concentration profiles and increases the dusty nanofluid's mass transfer efficiency. Wall friction reduction is used in oil refining and lowering of temperature profiles for cooling control and in manufacturing industries for improved heat transfer levels.

Abel and Shambajee [22]investigated "Effects of velocity, thermal and solutal slip boundary conditions on the flow and heat transfer of nanofluids past a linear stretching sheet with prescribed constant wall temperature". Here the effects of velocity, thermal and solutal slip boundary conditions on thenano-fluid flow and heat transfer with constant wall temperature are studied. Derived equations revels that, on increasing the velocity slip parameter (A) temperature, concentration increase whereas the skin friction coefficient decreases. As the thermal slip parameter (B) increases the temperature decreases. On increasing the velocity slip parameter (A) both Nusselt number and Sherwood number decrease whereas the concentration decreases with increase of Lewis number and temperature decreases with increase of Prandtl number. Ramanaiah et al [23] investigated the Sisko-nano-fluid convective heat and mass transfer flow through a nonlinear stretching plate with thermal radiation. Results obtained showed that, with the increase of thermophoresis parameter, Brownian motion parameter, thermal Biot number, Biot number concentration and thermal radiation parameter, the fluid temperature increases. Increased amount of Prandtlnumber reduces the temperature and concentration of the fluid. The concentration of fluids decreases with the parameter of Brownian motion increasing. With the increase of the thermal Biot number the local Nusselt number increases and decreases with the increase of the Biot number concentration. Similarly, the amount of Local Sherwood increases with an increase in Biot concentration, and decreases with an increase in the number of thermal Biot.

Ali et al [24] investigated the similarity solution of unsteady MHD boundary layer flow and heat transfer using the Buongiorno model through a wedge (which is moving) in a nano-fluid. The Falkner- Skan boundary-layer problem for a moving wedge immersed in a nano-fluid in presence of magnetic field was studied here. Results obtained revels that increase in velocity increases the magnetic field and pressure gradient. Heat transfer rate increases with an increase in the parameter of thermophoresis, Prandtlnumber andratio of velocity but decreases for Brownian diffusion. The concentration decreases with an increase in the parameter of thermophoresis, Lewisnumber and velocity-ratio but in case of Brownian diffusion the concentration of nanoparticles decreases upto $\eta < 1$ and then increases. Jafarimoghaddam et al [25] performed systematic surveys on the wedge flow of magneto-nano-fluids. For test the efficacy of nano-fluids against the pure base fluids, the new Eulerian model is adopted. Here the MHD wedge flow of Cu -Water nano-fluids was observed, subject to a more stringent physical field. The most practical finding of the investigation is that, under certain conditions (different magnetic field and different wedge geometries, cooling or heating applications, and different nanoparticles sizes), the efficacy of nano-fluids is highly conditional.

Hayat et al [26] studied analytically the magneto-hydrodynamic (MHD) squeezing flow of couple stress nanomaterial within two parallel plates. In this investigation important characteristics of thermophoresis and Brownian motion are discussed. Result shows that on increasing the value of squeezing parameter velocity increases whereas temperature and concentration decrease. On increasing values of Prandtl number, temperature and

concentration show opposite behaviour. Concentration and temperature show opposite behaviour with the change of thermophoresis parameter. Samantara et al [27] have considered a problem of dusty fluid passing through plane wall jet. They have considered that the fluid is not electrified by outer source rather the dust particles are electrified due to collision among themselves as well as with the wall of the jet. The governing system of nonlinear partial differential equations is solved by using finite difference method of non-uniform grid. They concluded that the electrification of particles reduces the velocity and temperature gradient, leading to reduction of skin friction and heat transfer. Agbaje et al [28] studied a new numerical approach to the flow and heat transfer of MHD stagnation point to a stretch plate. A new approach called the Spectral Perturbation Approach (SPM) has been introduced to solve the governing equations and to find numerical solutions for skin friction coefficient, Nusselt number, heat transfer rate, and profiles of velocity and temperature. The study shows that when standard perturbation methods fail to solve complex expansions, SPM is useful as an alternative approach to achieve numerical solutions. It is also widely used also for difficult expansions that cannot be analytically solved after the first approximation.

Madaki et al [29] studied the solutions of unsteady squeezing nanofluid flow between two parallel plates analytically and numerically. The factors like radiation, heat generation/absorption, and profiles of temperature were discussed in detail. Here the Runge-Kutta4th order method along with shooting method was adopted to test the accuracy. The results obtained both numerically and analytically agreed to the extent which is desired. All the related parameters were discussed and presented in tables and graphs. Sobamowo et al [30] investigated Magnetohydrodynamic squeezing of the nano-fluid flow analysis using parameter variation method under the influence of slip boundary conditions. Tests obtained showed that the velocity of the fluid increases under the influence of slip condition with the increase in magnetic field and decreases on increasing magnetic field parameter if there is no slip condition. Also, the fluid's velocity increases with the slip parameter and it decreases under the no-slip condition with an increase in the number of Reynolds. Sobamowo and Akinshilo [31] studied nano-fluid squeezing flow between two parallel plates under the influence of magnetic field. Analytical methods are used to investigate the nanofluid's squeezing phenomenon when the plates pass apart and when they come together. Parameter-like concentration of nanoparticles, Hartmann and Eckert parameter are discussed. The perturbation method (PM) has been discussed here to provide approximate analytical solution for nonlinear problems. The solutions obtained were used to investigate the effects of nanoparticles concentration, Eckert number, Hartmann number, temperature distribution and pressure gradient on the squeezing flow. The results obtained were compared with the results obtained through numerical techniques available in the existing literature and good agreements defined existing findings.

Kho et al [32] examined the radiative effects on MHD Casson-nano-fluid flow over a stretchable wall with mass and heat transfer. The thickness of the boundary layer is seen to increase in the temperature and concentration profiles but the velocity decreases as the parameter of Casson-nano-fluid, the magneticparameter and the parameter of porosity increase. With the growth of thermophoresis, temperature and concentration increase. Coefficient of skin friction and local Nusselt number deceases with a value increase of M . Local Nusselt number is decreasing and Sherwood number is increasing as the Nb and Nt increases. Mahatha et al [33] studied dissipative effects on MHD Nano-fluid stagnation point flow past a stretchy surface with melting. They concluded that heat transfer rate is induced by magnetic field, Brownian diffusion, thermophoretic diffusion, Lewis number and viscous dissipation while thermal diffusion and sheet melting reversely influence the heat transfer rate.

Mahatha et al [34] investigated dissipative effects of a heat-absorbing nano-fluid on MHD stagnation point flow through a stretchable surface with melting. Their concluding remarks are as follows:

- "Magnetic field and velocity ratio parameter are the reason for enhancement in skin friction while the other parameters are the cause for the decrease in skin friction".
- "Rate of heat transfer at the surface is getting enhanced by magnetic field, Brownian diffusion, thermophoretic diffusion, heat absorption, viscous dissipation, velocity ratio parameter, and Levis number while it is getting reduced by melting parameter, and thermal diffusion".

Mahato et al [35] carried out a research study on Melting heat transfer on magnetohydrodynamic (MHD) Nano-fluid heat radiation and chemical reaction flow through a stretchable surface. They find that heat transfer coefficient is a growing function of the parameter of velocity ratio, magnetic field, Brownian motion and thermophoresis diffusion, although it is a decreasing function of thermal diffusion, thermal radiation, sheet melting and chemical reaction.

REFERENCES

1. S. U. S.Choi and J. A. Eastman (1995). Enhancing thermal conductivity of fluids with nanoparticles: The Proceedings of the ASME International Mechanical Engineering Congress and Exposition, San Francisco, USA, ASME, FED 231/MD 66: 99-105.
2. S. U. S. Choi, Z. G. Zhang, W. Yu, F.E. Lockwood and E. A.Grulke (2001). Anomalously thermal conductivity enhancement in nanotube suspensions, Appl. Phys. Lett, 79: 2252-2254.
3. W.A. Khan and I. Pop (2010), "Boundary-layer flow of a nanofluid past a stretching sheet", *International Journal of Heat and Mass Transfer*, Vol. 53,pp. 2477–2483.
4. C.J. Ho, L.C. Wei, and Z.W. Li (2010), "An experimental investigation of forced convective cooling performance of a microchannel heat sink with Al2O3/water nanofluid", *Applied Thermal Engineering*, Vol.30, pp. 96–103.
5. M.A.A. Hamad (2011), "Analytical solution of natural convection flow of a nanofluid over a linearly stretching sheet in the presence of magnetic field", *International Communications in Heat and Mass Transfer*, Vol.38,pp. 487–492.
6. F.M. Hady, F. S. Ibrahim, S. M .A. Gaied, and M. R. Eid (2012), "Radiation effect on viscous flow of a nanofluid and heat transfer over a nonlinearly stretching sheet", *Nanoscale Research Letters*,
7. Cortell R: Effects of viscous dissipation and radiation on the thermal boundary layer over a non-linearly stretching sheet. Phys Lett A 2008, 372: 631-636.
8. T. G. Motsumi and O. D. Makinde, (2012), "Effects of thermal radiation and viscous dissipation on boundary layer flow of nanofluids over a permeable moving flat plate", *PhysicaScripta*, Scr.86, 045003 (8pp)
9. P. K. Singh, P.V. Harikrishna, T. Sundararajan , and S. K. Das, (2012), "Experimental and numerical investigation into the hydrodynamics of nanofluid in microchannels", *Experimental Thermal and Fluid Science*, Vol.42, pp. 174–186.
10. M. Kalteh, A. Abbassi, M.S. Avval , A. Frijns , A. Darhuber , and J. Harting , (2012), "Experimental and numerical investigation of nanofluid forced convection inside a wide microchannel heat sink", *Applied Thermal Engineering*, Vol.36, pp. 260-268
11. M.J. Uddin, W. A. Khan, and A. I. M. Ismail, (2012) "Scaling Group Transformation for MHD Boundary Layer Slip Flow of a Nanofluid over a Convectively Heated Stretching Sheet with Heat Generation", *Mathematical Problems in Engineering*.
12. O.D. Makinde, W.A. Khan, and Z.H. Khan, (2013), "Buoyancy effects on MHD stagnation point flow and heat transfer of a nanofluid past a convectively heated stretching/shrinking sheet", *International Journal of Heat and Mass Transfer*, Vol.62, pp. 526–533.
13. N. S. Akbar, S. Nadeem, R. U. Haq , and Z.H. Khan, (2013), "Radiation effects on MHD stagnation point flow of nano fluid towards a stretching surface with convective boundary condition", *Chinese Journal of Aeronautics*, Vol.26(6), pp. 1389–1397.
14. W.A. Khan, and I. Pop (2013), "Boundary Layer Flow Past a Wedge Moving in a Nanofluid", *Mathematical Problems in Engineering*, Vol 2013, Article ID 637285, 7 pages.
15. K. Das, P.R. Duariand, and P.K. Kundu, (2015), "Numerical simulation of nanofluid flow with convective boundary condition", *Journal of the Egyptian Mathematical Society*, Vol.23, pp. 435–439.
16. M.M.M. Hasan, M. Wahiduzzaman, and M.M. Alam, (2015), "MHD Radiative Heat and Mass Transfer Nanofluid Flow Past a Horizontal Stretching Sheet in a Rotating System", Vol.6, Issue 1.

17. M.R. Krishnamurthy, B.C. Prasannakumara, B.J. Gireesha, and R. S. R. Gorla, (2016), "Effect of chemical reaction on MHD boundary layer flow and melting heat transfer of Williamson nanofluid in porous medium", Vol. 19, pp. 53–61.
18. O.D. Makinde, and I.L. Animasaun, (2016) "Bioconvection in MHD nanofluid flow with nonlinear thermal radiation and quartic autocatalysis chemical reaction past an upper surface of a paraboloid of revolution", *International Journal of Thermal Sciences* , Vol. 109, pp. 159-171.
19. A. K. Pandey and M. Kumar, (2016), "Effect of viscous dissipation and suction/injection on MHD nanofluid flow over a wedge with porous medium and slip", *Alexandria Engineering Journal*, Vol. 55, pp. 3115–3123.
20. N. Kishan, C. Kalyani, M.C.K. Reddy, (2016), "MHD Boundary Layer Flow of a Nanofluid over an Exponentially Permeable Stretching S", *Trans. Phenom. Nano Micro Scales heet with radiation and heat Source/Sink*, Vol. 44, , 4(1), pp. 44-51.
21. N. Sandeep and M. S. Jagadeesh Kumar, (2016), "Heat and Mass Transfer in Nanofluid Flow over an Inclined Stretching Sheet with Volume Fraction of Dust and Nanoparticles", *"Journal of Applied Fluid Mechanics"*.Vol 9, pp. 2205-2215.
22. M.S. Abel and N.R.S. Shambajee, (2016), "Effects of velocity, thermal and solutal slip boundary conditions on the flow and heat transfer of nanofluids past a linear stretching sheet with prescribed constant wall temperature", *International Journal on Emerging Technologies*, Vol. 7, pp. 393-403.
23. G.V. Ramanaiah, M.S. Babu, M. Lavanyao, (2016), "Convective Heat and Mass Transfer Flow of Siskonanofluid Past a Nonlinear Stretching Sheet with Thermal Radiation", *International Refereed Journal of Engineering and Science*, Vol. 5, pp. 17-37.
24. M. Ali, M. A. Alim, R. Nasrin, M. S. Alam, and M. J. H. Munshi, (2017), "Similarity Solution of Unsteady MHD Boundary Layer Flow and Heat Transfer past a Moving Wedge in a Nanofluid using the Buongiorno Model", *Procedia Engineering*, Vol. 194, pp. 407 – 413.
25. A.Jafarimoghaddam, H. Aberouman, S. Aberoumand, A.A.A. Arani, and A. Habibollahzade, (2017), *Engineering Science and Technology, an International Journal*, Vol. 20, pp. 1515–1530.
26. T. Hayat, R. Sajjad, A. Alsaedi, T. Muhammada, and R. Ellahi, (2017), "On squeezed flow of couple stress nanofluid between two parallel plates", *Results in Physics*, Vol. 7, pp. 553–561.
27. T. N. Samantara, S.K. Mishra, and T.C. Panda "Numerical Modeling of Two Phase Jet Flow and Heat Transfer with Charged Suspended Particulate Matter (SPM)", *AMSE JOURNALS*-AMSE IIETA publication-2017-Series: Modelling B, Vol. **86**(4): 885 – 906
28. T.M. Agbaje, S. Mondal , Z.G. Makukula, S.S. Motsa, and P. Sibanda, (2018), "A new numerical approach to MHD stagnation point flow and heat transfer towards a stretching sheet", *Ain Shams Engineering Journal*, Vol 9, 233–243.
29. A.G. Madaki, R. Roslan, M.S. Rusiman, and C.S.K. Raju, (2018),"Analytical and numerical solutions of squeezing unsteady Cu and TiO2-nanofluid flow in the presence of thermal radiation and heat generation/absorption", *Alexandria Engineering Journal*, Vol 57, pp. 1033–1040.
30. M.G. Sobamowo, L.O. Jayesimi, and M.A. Waheed, (2018), "Magnetohydrodynamic squeezing flow analysis of nanofluid under the effect of slip boundary conditions using variation of parameter method", *Karbala International Journal of Modern Science*, Vol. 4, pp. 107-118.
31. M.G. Sobamowo, and A.T. Akinshilo, (2018), "On the analysis of squeezing flow of nanofluid between two parallel plates under the influence of magnetic field", *Alexandria Engineering Journal*, Vol. 57, pp. 1413–1423.
32. Y.B. Kho, A. Hussanan, N. M. Sari, Z. Ismail and M.Z. Salleh, (2018), "Thermal Radiation Effects on MHD with Flow Heat and Mass Transfer in CassonNanofluid over A Stretching Sheet", *MATEC Web of Conferences*, Vol. 150, 06036.
33. B. K. Mahatha, G. K. Mahato, and S. Nayak (2019), "Dissipative Effects on MHD Stagnation Point Nano-Fluid Flow past a Stretchable Surface with Melting" *Advances and Applications in Fluid Mechanics*, Volume 23, Number 1, pp. 97-118.

34. B. K. Mahatha, G. K. Mahato, and C. Jena (2019), "Dissipative Effects on MHD Stagnation Point Flow of a Heat Absorbing Nano-Fluid past a Stretchable Surface with Melting", *International Journal on Emerging Technologies*, Vol. 10 (2b), pp. 179-187.
35. G. K. Mahato, B. K. Mahatha and S. Samal (2019), "Melting Heat Transfer on Magnetohydrodynamic (MHD) Flow of a Heat Radiating and Chemically Reacting Nano-Fluid past a Stretchable Surface", *JP Journal of Heat and Mass Transfer*, Vol. 17, Issue 2, pp. 379-398.

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RESEARCH ARTICLE

Gallic Acid Possibly May Stall the Activity of the 2019-nCoV Main Protease

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ABSTRACT

In past two decades, the globe has faced many infectious disease outbreaks. 2019 Novel Corona-virus (2019-nCoV) or the severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) emerged as a global risk and put the entire globe into unrest. Unavailability of specific drug against the virus is more imperative. This demanding situation requires development of biomolecules for competent treatment against the SARS-CoV-2. The crystal structure of SARS-CoV-2 main protease (M^{pro}) may be used for fast *in silico* docking and novel pharmacophores can be discovered. This may result into identification of active bio-molecules largely phytochemicals. *In silico* Molecular Docking revealed that the phytochemical, Gallic acid effectively binds to the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, gallic acid.

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1,2]. SARS-CoV-2 belongs to the Beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3,4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1,5,6]. The virus is very contagious and infectious occurs through droplets from coughing and sneezing and touching infected surface. Its genome comprises of nearly 30,000 nucleotides and encoded by 4 structural proteins. Those are Nucleocapsid protein, Membrane protein, Envelope protein, and Spike

protein. The virus possesses a positive single stranded RNA. It attacks human cells and converted them into factories of viruses. The capsid protein helps in its replication and transcription. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [7]. SARS-CoV-2 main protease can be beleaguered for developing antibodies, diagnostics and vaccines. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8,9,10]. Moreover, M^{pro} can also be an effectual target to diminish the viral replications within the host cells since it facilitates the synthesis of functional viral proteins. The effectiveness of traditional medications on the restriction of COVID-19 growth does not have any scientific back up as of now, since the underlying molecular mechanisms are unclear. The phytochemicals are fundamentally bioactive compounds and has the potential to amend cellular physiology. Here, we report that Gallic acid, a phytochemical, mostly enriched in some selected plants binds into the active site of the SARS-CoV-2 main protease as revealed by the *in silico* molecular docking and thus further studies may reveal the effectiveness of Gallic acid to be used as COVID-19 therapeutics.

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6M03 (Fig. 1). The SDF accession CHEBI:30778 corresponding to the Gallic acid (Fig. 2) was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. -CDOCKER Energy and -CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the -CDOCKER Energy and -CDOCKER Interaction Energy are considered to be the most favourable [12].

RESULTS AND DISCUSSION

Through the process of molecular docking i.e. *in silico* molecular docking, some phytochemicals have shown their effectiveness against the particular disease. As the crystal structure of SARS-CoV-2 has been solved i.e. main protease (M^{pro}), it can be considered as the root way for the screening of inhibitory ligands to detect bioactive molecules. Through *in silico* molecular docking, Gallic acid has remarkably shown the effectiveness against COVID-19 by binding to the active sites of SARS-CoV-2 main protease (M^{pro}). It was found that Gallic acid, a common phytochemical, specifically binds to the active pocket of the SARS-CoV-2 M^{pro} (Fig. 3), as apparent from higher -CDOCKER energy and -CDOCKER interaction energy. Since, simple active biomolecule like Gallic acid effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Gallic acid and eventually can be used in the pharmaceutical sectors. Chemical synthesis of Gallic acid can be cost effective as compared to the isolation process from specific plants.

CONCLUSION AND FUTURE PERSPECTIVES

As the coronavirus outbreak became the nightmare for the whole human society and the devastation caused by it is unpredictable and beyond imagination, the world has not left with enough time to discover a new drug or vaccine for it due to the requirement of sufficient time. Due to its highly contagious nature, it is considered as global pandemic within no time by taking many lives of people. But future studies on Gallic acid may become the building

block for the medication and treatment against the SARS-CoV-2. The current *in silico* molecular docking based study reveals that Gallic acid can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Gallic acid is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like Gallic acid which can be employed for designing novel therapeutics.

Author contribution statement

KBS and GKP conceived the idea. AS, GKP, PKP, SKS, CR performed the experiments. KBS, GKP and CR analyzed the data. All authors have significant contribution in drafting the manuscript

Funding

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ACKNOWLEDGEMENTS

Authors are thankful to the administration and management of Centurion University of Technology and Management, Odisha, India for providing necessary facilities to conduct the experiment.

Conflict of interest

The authors declare that they have no conflict of interest.

REFERENCES

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3. Lu R, Zhao X, Li J, et al. 2020. Genomic characterisation and epidemiology of 2019 novel coronavirus: implications for virus origins and receptor binding. Lancet 395, 565-574.
4. Wu F, Zhao S, Yu B, et al. 2020. A new coronavirus associated with human respiratory disease in China. Nature 579, 265-269.
5. Chan JFW, Yuan S, Kok KH, et al. 2020. A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster. Lancet 395, 514-523.
6. Li Q, Guan X, Wu P, et al. 2020. Early Transmission Dynamics in Wuhan, China, of Novel Coronavirus–Infected Pneumonia. N Engl J Med 1-9.
7. Liu W, Morse JS, Lalonde T, Xu S. 2020. Learning from the Past: Possible Urgent Prevention and Treatment Options for Severe Acute Respiratory Infections Caused by 2019-nCoV. Chem Bio Chem, 730-738.
8. Wrapp D, Wang N, Corbett KS, et al. 2020. Cryo-EM structure of the 2019-nCoV spike in the prefusion conformation. Science 1263, 1260-1263.
9. Lung Jrhau, Yu-Shih Lin, Yao-Hsu Yang, et al. 2020. The potential chemical structure of anti-SARS-CoV-2 RNA-dependent RNA polymerase. J Med Virol 0-1.
10. Ton A-T, Gentile F, Hsing M, et al. 2020. Rapid Identification of Potential Inhibitors of SARS- CoV-2 Main Protease by Deep Docking of 1.3 Billion Compounds. Mol Inform 1-18.
11. Dassault Systèmes BIOVIA, DISCOVERY STUDIO, San Diego: Dassault Systèmes, 2020.
12. Panigrahi Gagan Kumar, Sahoo Shraban Kumar and Satapathy Kunja Bihari. 2020. In silico Molecular Docking-Based Screening of Phytochemicals Targeted against Glypican-1. IJONS. 59(10), 18708-18712.

Table 1: -CDOCKER ENERGY and -CDOCKER INTERACTION ENERGY values generated for the interaction of Gallic acid with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand		Receptor		Interaction Status		
SDF accession	Phytochemical	Protein	PDB accession	Docking Result	CDOCKER ENERGY	CDOCKER INTERACTION ENERGY
CHEBI:30778	Gallic acid	COVID-19 Main Protease	6M03	POSITIVE	18.34	17.58

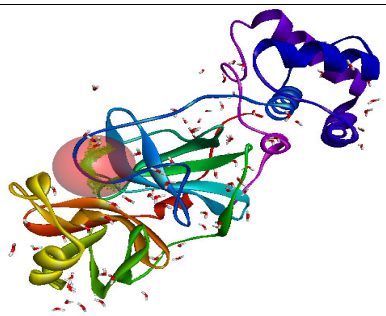

Fig. 1: 3-D Structure of the SARS-CoV-2 M^{pro} showing the active site of the protein.

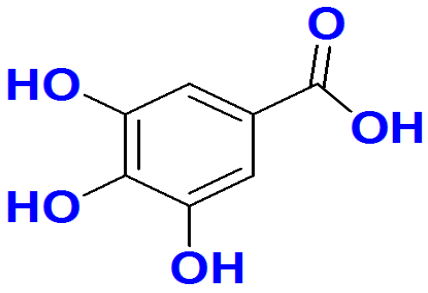

Fig. 2: Chemical structure of Gallic acid

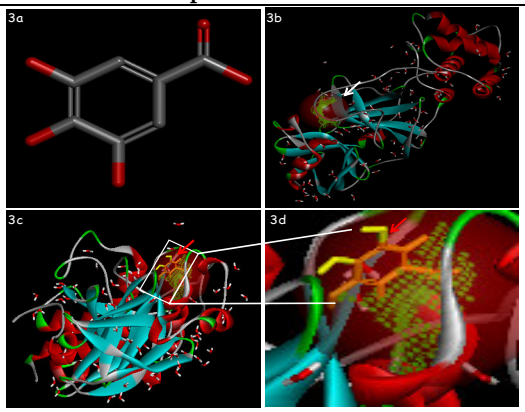

Fig. 3: The active site of the SARS-CoV-2 main protease (M^{pro}) interacts with Gallic acid. 3a: Phytochemical, Gallic acid. 3b: Free form of the M^{pro}. 3c: M^{pro} associated with the ligand, Gallic acid. 3d: Magnified image showing the association of the Gallic acid with the M^{pro}. (The white coloured arrow and the red coloured arrow indicate the active site of the M^{pro} and binding of Gallic acid respectively).

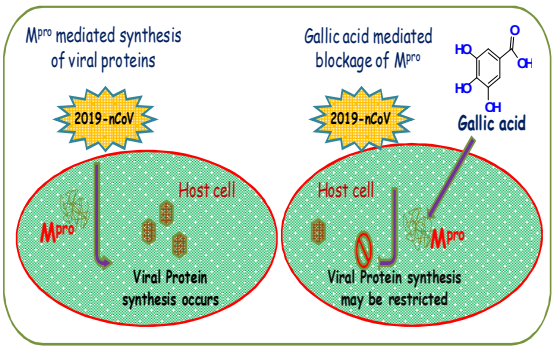

Fig. 4: Gallic acid may inhibit the activity of COVID-19 M^{pro}.

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RESEARCH ARTICLE

In Silico Analysis Reveals the Binding of Daidzen to Active Pocket of the SARS-Cov-2 Main Protease

Gagan Kumar Panigrahi[1], Annapurna Sahoo[2], Pradip Kumar Prusty[1], Shraban Kumar Sahoo[1], Chittaranjan Routray[1] and Kunja Bihari Satapathy[1]*

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ABSTRACT

2019 Novel corona-virus (2019-nCoV) came up as a worldwide risk factor and put the entire human species into unrest. Till date, specific drug against the virus is not available. The current state of affair demands the development of anti-viral molecules against 2019-nCoV. The three dimensional structure of SARS-CoV-2 main protease (M^{pro}) can be used for high throughput screening of potential chemicals by *in silico* docking. This may result into identification of active biomolecules like phytochemicals. *In silico* Molecular Docking revealed that the phytochemical, Daidzein which belongs to isoflavone category effectively binds to the active pocket of the severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) or the 2019-nCoV main protease.

Keywords: 2019-nCoV, SARS-CoV-2 main protease, SARS-CoV-2, *in silico*, molecular docking, phytochemicals.

INTRODUCTION

Owing to the spread of 2019-nCoV which resulted into the pandemic situation represents a severe public health crisis. Outbreak of this human pathogen emerged in the city of Wuhan, and resulted to human illness, termed as COVID-19 [1,2]. SARS-CoV-2 belongs to the Beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [3,4]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1,5,6]. Novel coronavirus induces respiratory disease and around 10-15% patients have acute respiratory distress syndrome, which is triggered primarily by cytokines. It has been reported that the neutrophilic

extracellular traps (NET) contributes to organ damage and mortality in COVID-19. NET is also linked to pulmonary diseases, thrombosis, mucous secretions and cytokine production. NETs may be well targeted to reduce the clinical severity of COVID-19. The severity of COVID-19 depends upon the pandemic spread and unprecedented pressure on health care system. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) can be effectively used for screening specific ligands [7]. M^{pro} and other known viral proteins are defining features which allow the virus to enter and infect the host cell [8,9,10]. M^{pro} can be an effective target to diminish the viral replications within the host cells since it facilitates the synthesis of functional viral proteins. Effective curative measures against SARS-CoV-2 are lacking. Phytochemicals which are fundamentally bioactive compounds and has the potential to amend cellular physiology may be screened against the viral proteins. Here, we report that Daidzein, a phytochemical binds to the active site of the SARS-CoV-2 main protease as revealed by the *in silico* molecular docking and thus further studies may reveal the effectiveness of Daidzein to be used as COVID-19 therapeutics.

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6M03 (Fig. 1). The SDF accession CHEBI:28197 corresponding to the Daidzein (Fig. 2) was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. -CDOCKER Energy and -CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the -CDOCKER Energy and -CDOCKER Interaction Energy are considered to be the most favourable [11,12].

RESULTS AND DISCUSSION

It was found that Daidzein specifically binds to the active pocket of the SARS-CoV-2 M^{pro} (Fig. 3), as apparent from higher -CDOCKER energy and -CDOCKER interaction energy (Table 1). Since, Daidzein effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Daidzein. Chemical synthesis of Daidzein can be cost effective as compared to the isolation process from specific plants.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that Daidzein can target the reported SARS-CoV-2 M^{pro} (Fig. 4). It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like Daidzein is commercially available and thus may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like Daidzein which can be employed for designing novel therapeutics.

Author contribution statement

KBS and GKP conceived the idea. AS, GKP, PKP, SKS, CR performed the experiments. KBS, GKP and SKS analyzed the data. All authors have significant contribution in drafting the manuscript.

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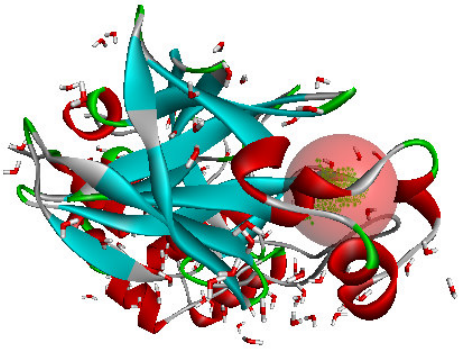

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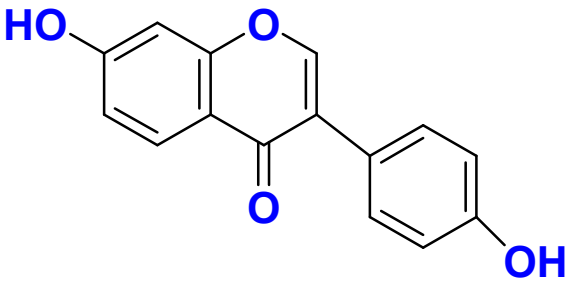

Fig. 2: Chemical structure of Daidzein

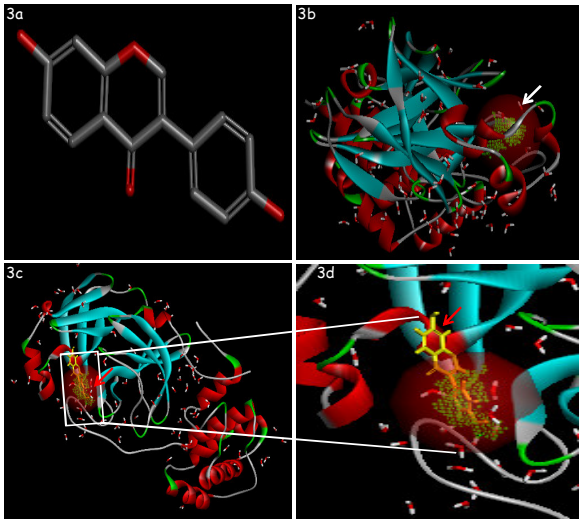

Fig. 3: The active site of the SARS-CoV-2 main protease (M^{pro}) interacts with Daidzein. 3a: Phytochemical, Daidzein. 3b: Free form of the M^{pro}. 3c: M^{pro} associated with the ligand, Daidzein. 3d: Magnified image showing the association of the Daidzein with the M^{pro}. (The white coloured arrow and the red coloured arrow indicate the active site of the M^{pro} and binding of Daidzein respectively).

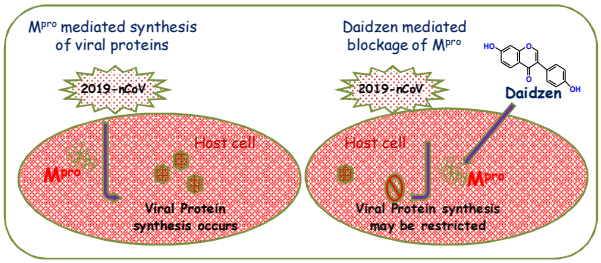

Fig. 4: Daidzen may act against the COVID-19 M^{pro}.

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RESEARCH ARTICLE

Kaempferol against SARS-Cov-2 Main Protease: A Molecular Docking Study

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ABSTRACT

The emerging 2019 Novel coronavirus (2019-nCoV) threatens public health. 2019-nCoV is also referred to as severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2). Within no time 2019-nCoV emerged as a global risk and was declared as pandemic. Specific drug against the virus is yet to be discovered. Development of biomolecules for proficient treatment against severe acute SARS-CoV-2 is challenging. The solved crystal structure of SARS-CoV-2 main protease (M^{pro}) can be used as one of the primary target molecules and possible inhibitory ligands may be screened using *in silico* docking. Primarily phytochemicals can be screened to detect any potential bioactive molecules. *In silico* molecular docking revealed that the phytochemical, Kaempferol belonging to the flavanoid group of phytochemical may effectively binds to the active site of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, *in silico* docking, phytochemicals.

INTRODUCTION

Corona viruses are the group of viruses, which are able to cause diseases in both animal and humans. One of the best examples of previously known coronavirus is severe acute respiratory syndrome (SARS) and the virus strain is known as SARS-CoV. Further new strains of Corona virus are identified, known as severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). This virus is responsible for causing coronavirus disease 19 (COVID-19). The new coronavirus has spread very rapidly in different parts of the world. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1, 2]. SARS-CoV-2 belongs to the beta corona-virus genus [3,4]. On 11th March, 2020 the World Health Organization (WHO)

declared that COVID-19 as a pandemic. A pandemic occurs when, the disease that people are not immune to spread across the large region. Countries including United States of America, Italy had largest outbreak outside China with increased number of infected people leading to death of individuals [1,5,6]. The pandemic ratio changes very rapidly with fresh data collected on the basis of chemical and serological characteristics of affected case being reported every day. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an outstanding ground for screening specific ligands [7]. Reportedly, M^{pro} and other known viral proteins infect the respiratory tract [8,9,10]. Moreover, M^{pro} can also be an effectual target to diminish the viral replications within the host cells since it facilitates the synthesis of functional viral proteins. Here, we report that Kaempferol binds into the active site of the SARS-CoV-2 main protease as revealed by the *in silico* molecular docking and thus further studies may reveal the effectiveness of Kaempferol to be used as COVID-19 therapeutics.

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6M03 (Fig. 1). The SDF accession CHEBI:28499 corresponding to the Kaempferol (Fig. 2) was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. -CDOCKER Energy and -CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the -CDOCKER Energy, -CDOCKER Interaction Energy and a diminutive difference between the -CDOCKER Energy and -CDOCKER Interaction Energy are considered to be the most favourable [11,12].

RESULTS AND DISCUSSION

It was found that Kaempferol specifically binds to the active pocket of the SARS-CoV-2 M^{pro} (Fig. 3), as apparent from higher -CDOCKER energy and -CDOCKER interaction energy (Table 1). Since, simple active biomolecule like Kaempferol effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Kaempferol and eventually can be used in the pharmaceutical sector. Chemical synthesis of Kaempferol can be cost effective as compared to the isolation process from specific plants.

CONCLUSION AND FUTURE PERSPECTIVES

Among the large family of corona viruses, about hundreds of these viruses circulate in animals. Among them only seven infect humans and cause symptoms of common cold. SARS coronavirus emerged in 2002 and was controlled by public health measures. But MERS which emerged in the year 2012, still exists in camels, it can also affect humans who come in contact with infected camels. The 2019-nCoV reported from the city of Wuhan, has now spread into more than 200 countries. The World Health Organization declared novel coronavirus outbreak "a public health emergency of international concern" on 30th January. On 11th March WHO declared COVID-19 epidemic a pandemic. The current *in silico* molecular docking based study reveals that Kaempferol can target the reported SARS-CoV-2 M^{pro} (Fig. 4). It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Pharmacophores developed from Kaempferol can be synthesized and may be effective against SARS-CoV-2 M^{pro}. Essentially, this study makes an attempt to reveal simple phytochemicals like Kaempferol which may be employed for designing novel therapeutics and hopefully blunt the spread of this deadly virus.

Author contribution statement

KBS and GKP conceived the idea. AS, GKP, PKP, SKS, CR performed the experiments. KBS, GKP and CR analyzed the data. All authors have significant contribution in drafting the manuscript.

Funding

The present study was financially supported by Centurion University of Technology and Management, Odisha, India.

ACKNOWLEDGEMENTS

Authors are thankful to the administration and management of Centurion University of Technology and Management, Odisha, India for providing necessary facilities to conduct the experiment.

Conflict of interest

The authors declare that they have no conflict of interest.

REFERENCES

1. Chen N, Zhou M, Dong X, et al. 2020. Epidemiological and clinical characteristics of 99 cases of 2019 novel coronavirus pneumonia in Wuhan, China: a descriptive study. Lancet 395, 507-513.
2. Huang C, Wang Y, Li X, et al. 2020. Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China. Lancet 395, 497-506. https://doi.org/10.1016/S0140-6736(20)30183-5.
3. Lu R, Zhao X, Li J, et al. 2020. Genomic characterisation and epidemiology of 2019 novel coronavirus: implications for virus origins and receptor binding. Lancet 395, 565-574.
4. Wu F, Zhao S, Yu B, et al. 2020. A new coronavirus associated with human respiratory disease in China. Nature 579, 265-269.
5. Chan JFW, Yuan S, Kok KH, et al. 2020. A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster. Lancet 395, 514-523.
6. Li Q, Guan X, Wu P, et al. 2020. Early Transmission Dynamics in Wuhan, China, of Novel Coronavirus-Infected Pneumonia. N Engl J Med 1-9.
7. Liu W, Morse JS, Lalonde T, Xu S. 2020. Learning from the Past: Possible Urgent Prevention and Treatment Options for Severe Acute Respiratory Infections Caused by 2019-nCoV. Chem Bio Chem 730-738.
8. Wrapp D, Wang N, Corbett KS, et al. 2020. Cryo-EM structure of the 2019-nCoV spike in the prefusion conformation. Science 1263,1260-1263.
9. Lung Jrhau, Yu-Shih Lin, Yao-Hsu Yang, et al. 2020. The potential chemical structure of anti-SARS-CoV-2 RNA-dependent RNA polymerase. J Med Virol 0-1.
10. Ton AT, Gentile F, Hsing M, et al. 2020. Rapid Identification of Potential Inhibitors of SARS- CoV-2 Main Protease by Deep Docking of 1.3 Billion Compounds. Mol Inform 1-18.
11. Dassault Systèmes BIOVIA, DISCOVERY STUDIO, San Diego: Dassault Systèmes, 2020.
12. Panigrahi Gagan Kumar, Sahoo Shraban Kumar and Satapathy Kunja Bihari. 2020. In silico Molecular Docking-Based Screening of Phytochemicals Targeted against Glypican-1. IJONS. 59(10),18708-18712.

Table 1: -CDOCKER ENERGY and -CDOCKER INTERACTION ENERGY values generated for the interaction of Kaempferol with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand		Receptor		Interaction Status		
SDF accession	Phytochemical	Protein	PDB accession	Docking Result	CDOCKER ENERGY	CDOCKER INTERACTION ENERGY
CHEBI:28499	Kaempferol	COVID-19 Main Protease	6M03	POSITIVE	15.71	22.01

Fig. 1: 3-D Structure of the SARS-CoV-2 M^{pro} showing the active site of the protein.

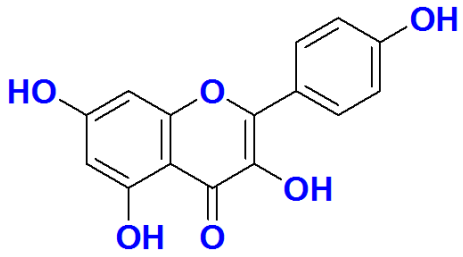

Fig. 2: Chemical structure of Kaempferol

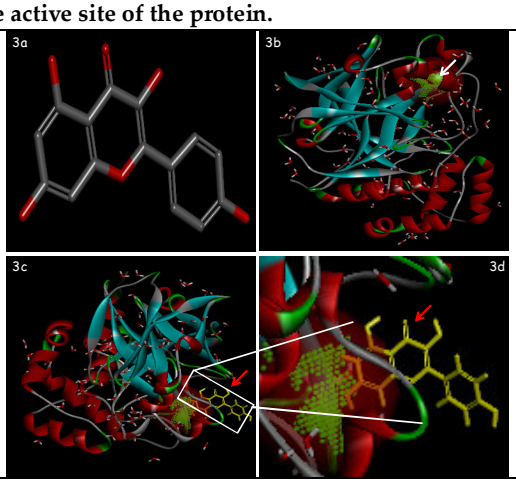

Fig. 3: The active site of the SARS-CoV-2 main protease (M^{pro}) interacts with Kaempferol. 3a: Phytochemical, Kaempferol. 3b: Free form of the M^{pro}. 3c: M^{pro} associated with the ligand, Kaempferol. 3d: Magnified image showing the association of the Kaempferol with the M^{pro}. (The white coloured arrow and the red coloured arrow indicate the active site of the M^{pro} and binding of Kaempferol respectively).

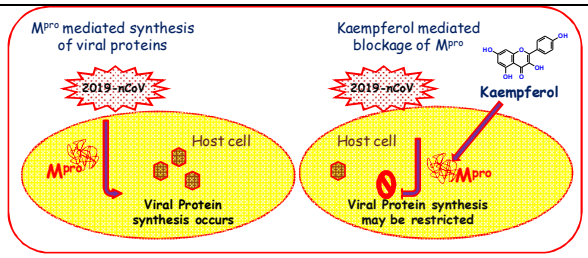

Fig. 4: Kaempferol may inhibit the activity of COVID-19 M^{pro}.

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RESEARCH ARTICLE

Plant Organosulfides against 2019-nCoV Main Protease: A Molecular Docking Study

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ABSTRACT

The emerging 2019 Novel coronavirus (2019-nCoV) threatens public health. 2019-nCoV is also referred to as severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2). Within no time it emerged as a global risk and was declared as pandemic. Specific drug against the virus is yet to be discovered. Development of biomolecules for proficient treatment against severe acute SARS-CoV-2 is challenging. The solved crystal structure of SARS-CoV-2 main protease (M^{pro}) can be used as one of the primary target molecule and possible inhibitory ligands may be screened using *in silico* docking. Primarily phytochemicals can be screened to detect any potential bioactive molecules. *In silico* molecular docking revealed that the phytochemicals, benzyl isothiocyanate and phenyl isothiocyanate belonging to the organosulfide group of phytochemicals may effectively binds to the active site of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, *in silico* docking, phytochemicals, organosulfides. .

INTRODUCTION

Numerous members of the family Coronaviridae continuously circulate in the human population and usually cause mild respiratory disease [1]. Whereas, the severe acute respiratory syndrome Coronavirus (SARS-CoV) and the Middle East Respiratory Syndrome Coronavirus (MERS-CoV) are transmitted from animals to humans resulting into SARS and MERS, respectively [2]. Natural reservoir hosts for SARS-CoV were Chinese horseshoe bats [3,4]. Intermediate hosts like civet cats and raccoon dogs, which are habitually sold as food sources in Chinese wet markets mediated the human transmission [5]. At present, no precise antivirals or approved vaccines are available to combat

the current pandemic situation. Presently, conventional control measures, including travel restrictions and self-quarantine are practiced. The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. This pathogen emerged from the city of Wuhan and resulted into this scariest situation, COVID-19 [6]. SARS-CoV-2 belongs to the beta corona-virus genus, closely related to the previously identified severe acute respiratory syndrome corona-virus (SARS-CoV) [7,8]. Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [9,10,11]. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [12]. SARS-CoV-2 main protease can be beleaguered for developing antibodies, diagnostics and vaccines. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [13,14,15]. Moreover, M^{pro} can also be an effectual target to diminish the viral replications within the host cells since it facilitates the synthesis of functional viral proteins. The effectiveness of traditional medications on the restriction of COVID-19 growth does not have any scientific back up as of now, since the underlying molecular mechanisms are unclear. The phytochemicals are fundamentally bioactive compounds and has the potential to amend cellular physiology. Here, we report that benzyl isothiocyanate and phenyl isothiocyanate, a mostly enriched in some selected plants bind into the active site of the SARS-CoV-2 main protease as revealed by the *in silico* molecular docking and thus further studies may reveal the effectiveness of benzyl isothiocyanate and phenyl isothiocyanate to be used as COVID-19 therapeutics.

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6M03 (Fig. 1). The SDF accession CHEBI:17484 corresponding to the benzyl isothiocyanate and CHEBI:85103 corresponding to the phenyl isothiocyanate (Fig. 2) was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [16] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. -CDOCKER Energy and -CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the -CDOCKER Energy and -CDOCKER Interaction Energy are considered to be the most favourable [17].

RESULTS AND DISCUSSION

It was found that phenyl isothiocyanate and benzyl isothiocyanate binds effectively to the active pocket of the SARS-CoV-2 M^{pro} (Fig. 3 and Fig. 4), as apparent from higher -CDOCKER energy and -CDOCKER interaction energy. Since, simple active biomolecule like benzyl isothiocyanate and phenyl isothiocyanate effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of benzyl isothiocyanate and phenyl isothiocyanate and eventually can be used in the pharmaceutical sector. Chemical synthesis of benzyl isothiocyanate and phenyl isothiocyanate like molecules can be cost effective as compared to the isolation process from specific plants.

CONCLUSION AND FUTURE PERSPECTIVES

The current *in silico* molecular docking based study reveals that benzyl isothiocyanate and phenyl isothiocyanate can effectively target the SARS-CoV-2 M^{pro} (Fig. 5). It would be exceedingly notable being confirmed *in vivo*. It is crucial

to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemicals like benzyl isothiocyanate and phenyl isothiocyanate may be effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemicals like benzyl isothiocyanate and phenyl isothiocyanate which can be employed for designing novel therapeutics.

Author contribution statement

KBS, GKP and AS conceived the idea. AS, GKP, PKP, SKS, CR performed the experiments. KBS, GKP and AS analyzed the data. All authors have significant contribution in drafting the manuscript.

Funding

The present study was financially supported by Centurion University of Technology and Management, Odisha, India.

ACKNOWLEDGEMENTS

Authors are thankful to the administration and management of Centurion University of Technology and Management, Odisha, India for providing necessary facilities to conduct the experiment.

Conflict of interest

The authors declare that they have no conflict of interest.

REFERENCES

1. Corman VM, Lienau J, and Witzenrath M. 2019. Coronaviruses as the cause of respiratory infections. Internist (Berl.) 60, 1136-1145.
2. Fehr AR, Channappanavar R, and Perlman S. 2017. Middle East Respiratory Syndrome: Emergence of a Pathogenic Human Coronavirus. Annu. Rev. Med. 68, 387–399.
3. Lau SK, Woo PC, Li KS, Huang Y, et al. 2005. Severe acute respiratory syndrome coronavirus-like virus in Chinese horseshoe bats. Proc. Natl. Acad. Sci. USA 102, 14040-14045.
4. Li F, Li W, Farzan M, and Harrison SC. 2005. Structure of SARS coronavirus spike receptor-binding domain complexed with receptor. Science 309, 1864-1868.
5. Guan Y, Zheng BJ, He YQ, et al. 2003. Isolation and characterization of viruses related to the SARS coronavirus from animals in southern China. Science 302, 276-278.
6. 6. Chen N, Zhou M, Dong X, et al. 2020. Epidemiological and clinical characteristics of 99 cases of 2019 novel coronavirus pneumonia in Wuhan, China: a descriptive study. Lancet 39, 507-513.
7. Huang C, Wang Y, Li X, et al. 2020. Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China. Lancet 395, 497-506. https://doi.org/10.1016/S0140-6736(20)30183-5.
8. Lu R, Zhao X, Li J, et al. 2020. Genomic characterisation and epidemiology of 2019 novel coronavirus: implications for virus origins and receptor binding. Lancet 395, 565-574.
9. Wu F, Zhao S, Yu B, et al. 2020. A new coronavirus associated with human respiratory disease in China. Nature 579, 265-269.
10. Chan JFW, Yuan S, Kok KH, et al. 2020. A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster. Lancet 395, 514-523.
11. Li Q, Guan X, Wu P, et al. 2020. Early Transmission Dynamics in Wuhan, China, of Novel Coronavirus–Infected Pneumonia. N Engl J Med 1-9.
12. Liu W, Morse JS, Lalonde T, Xu S. 2020. Learning from the Past: Possible Urgent Prevention and Treatment Options for Severe Acute Respiratory Infections Caused by 2019-nCoV. Chem Bio Chem 730-738.
13. Wrapp D, Wang N, Corbett KS, et al. 2020. Cryo-EM structure of the 2019-nCoV spike in the prefusion conformation. Science 1263,1260-1263.
14. Lung Jrhau, Yu-Shih Lin, Yao-Hsu Yang, et al. 2020. The potential chemical structure of anti-SARS-CoV-2 RNA-

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15. Ton AT, Gentile F, Hsing M, et al. 2020. Rapid Identification of Potential Inhibitors of SARS- CoV-2 Main Protease by Deep Docking of 1.3 Billion Compounds. Mol Inform 1-18.
16. Dassault Systèmes BIOVIA, DISCOVERY STUDIO, San Diego: Dassault Systèmes, 2020.
17. Panigrahi Gagan Kumar, Sahoo Shraban Kumar and Satapathy Kunja Bihari. 2020. In silico Molecular Docking-Based Screening of Phytochemicals Targeted against Glypican-1. IJONS 59(10),18708-18712.

Table 1: -CDOCKER ENERGY and -CDOCKER INTERACTION ENERGY values generated for the interaction of Plant organosulfides (Benzyl isothiocyanate and Phenyl isothiocyanate) with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand		Receptor		Interaction Status		
SDF accession	Phytochemical (Organosulfides)	Protein	PDB accession	Docking Result	CDOCKER ENERGY	CDOCKER INTERACTION ENERGY
		COVID-19 Main Protease (M^{pro})	6M03			
CHEBI:17484	Benzylisothiocyanate			POSITIVE	11.54	13.34
CHEBI:85103	Phenyl isothiocyanate			POSITIVE	13.76	16.31

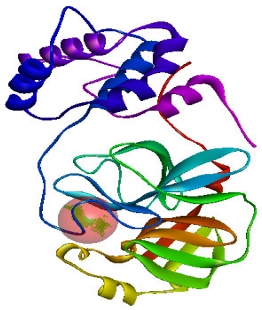

Fig. 1: 3-D Structure of the SARS-CoV-2 M^{pro} showing the active site of the protein.

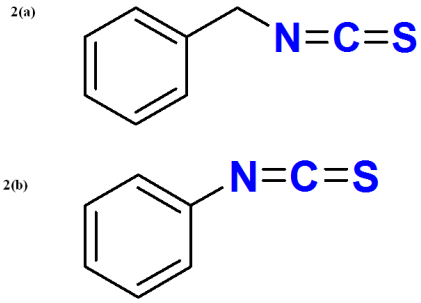

Fig. 2: Chemical structure of (a): benzyl isothiocyante and (b): phenyl isothiocyanate

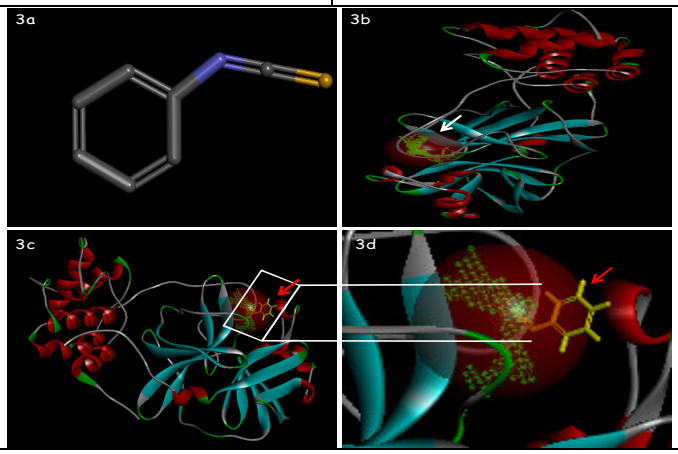

Fig. 3: The active site of the SARS-CoV-2 main protease (M^{pro}) interacts with Phenyl isothiocyanate. 3a: Phytochemical, Phenyl isothiocyanate. 3b: Free form of the M^{pro}. 3c: M^{pro} associated with the ligand, Phenyl isothiocyanate. 3d: Magnified image showing the association of the Phenyl isothiocyanate with the M^{pro}. (The white coloured arrow and the red coloured arrow indicate the active site of the M^{pro} and binding of Phenyl isothiocyanate respectively).

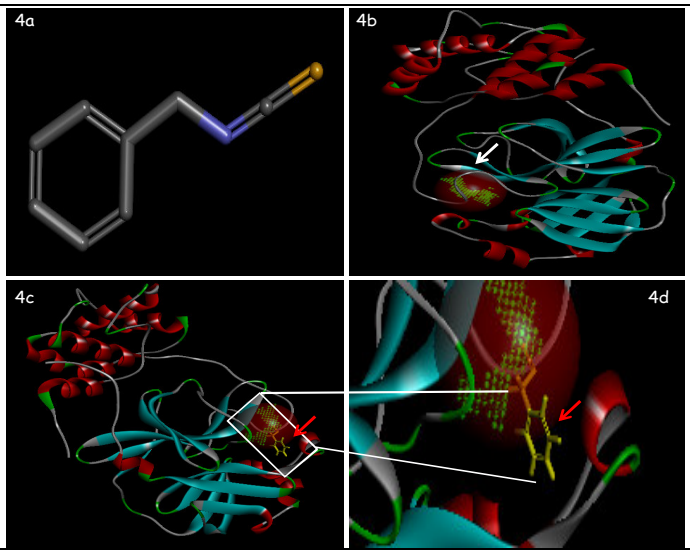

Fig. 4 : The active site of the SARS-CoV-2 main protease (M^{pro}) interacts with Benzyl isothiocyanate. 4a: Phytochemical, Benzyl isothiocyanate. 4b: Free form of the M^{pro}. 4c: M^{pro} associated with the ligand, Benzyl isothiocyanate. 4d: Magnified image showing the association of the Benzyl isothiocyanate with the M^{pro}. (The white coloured arrow and the red coloured arrow indicate the active site of the M^{pro} and binding of Benzyl isothiocyanate respectively).

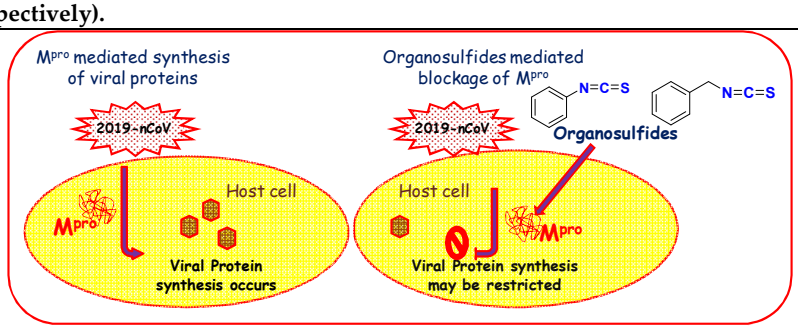

Fig. 5: Plant organosulfides may act against the COVID-19 M^{pro}.

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RESEARCH ARTICLE

The Phytochemical Alliin may Inhibit the Activity of the SARS-CoV-2 Main Protease

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ABSTRACT

The deadly infectious 2019 Novel corona-virus (2019-nCoV) also referred to as severe acute respiratory syndrome Corona-virus 2 (SARS-CoV-2) that took stem in Wuhan, China has spread all over the globe within no time. It is the cause of the increasing death rate of people. This challenging situation requires development of pharmacophore for efficient treatment against severe acute SARS-CoV-2. The available crystal structure of SARS-CoV-2 main protease (M^{pro}) can be used effectively for fast *in silico* docking. This may result into identification of active biomolecules including phytochemicals. *In silico* Molecular Docking revealed that the phytochemical, Alliin effectively binds to the active pocket of the SARS-CoV-2 main protease.

Keywords: 2019-nCoV, SARS-CoV-2, SARS-CoV-2 main protease, docking, phytochemicals, Alliin.

INTRODUCTION

The pandemic situation caused due to the 2019-nCoV represents a severe public health calamity across the globe. The city of Wuhan was the epicentre where the outbreak of this human pathogen emerged, and resulted to human ailment, termed as COVID-19 [1,2]. Coronavirus belongs to the family of Coronaviridae including 4 genera i.e. Alpha coronavirus, Beta coronavirus, Delta coronavirus, Gamma coronavirus. Among these, Beta coronavirus are severe acute respiratory syndrome coronavirus (SARS-CoV) and Middle East respiratory syndrome corona virus (MERS-Cove), which have engulfed more than 10,000 people around the globe in past two decades. SARS-CoV-2 belongs to Beta corona virus comprising of a positive single stranded RNA genome having 29,903 base pairs [3, 4]. These also show the characteristics of having genes encoding 3C-like proteins, RNA dependant RNA polymerase, 2 ′-O-ribose methyltransferase, spike protein, envelope protein, nucleocapsid phosphor protein and several unknown proteins.

Public Health Emergency of International Concern (PHEIC) was declared by the World Health Organization (WHO) owing to its fast rate of transmission within the humans [1,5,6]. The virus shows the symptoms such as fever, dry cough and difficulty in breathing. However, the treatment cannot be achieved by developing drugs against at this current time as it will take many years. Thus a strategy of rapid application of drug is necessary at this very moment. Crystal structure of the SARS-CoV-2 main protease (M^{pro}) proves to be an exceptional ground for screening specific ligands [7]. SARS-CoV-2 main protease can be beleaguered for developing antibodies, diagnostics and vaccines. Reportedly, M^{pro} and other known viral proteins are defining features paving the path of virus from entry to infection in the host cell [8,9,10]. Moreover, M^{pro} can also be an effectual target to diminish the viral replications within the host cells since it facilitates the synthesis of functional viral proteins. The effectiveness of traditional medications on the restriction of COVID-19 growth does not have any scientific back up as of now, since the underlying molecular mechanisms are unclear. The phytochemicals are fundamentally bioactive compounds and has the potential to amend cellular physiology. Here, we report that Alliin, a phytochemical mostly enriched in some selected plants binds into the active site of the SARS-CoV-2 main protease as revealed by the *in silico* molecular docking and thus further studies may reveal the effectiveness of Alliin to be used as COVID-19 therapeutics.

METHODS

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of M^{pro} was accessed from Protein Data Bank accession 6M03 (Fig. 1). The SDF accession CHEBI:2596 corresponding to the Alliin (Fig. 2) was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking method [11] was used for molecular docking. The catalytic pocket of the M^{pro} protein was specified and targeted for binding of the ligand. -CDOCKER Energy and -CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the -CDOCKER Energy and -CDOCKER Interaction Energy are considered to be the most favourable [12].

RESULTS AND DISCUSSION

It was found that Alliin specifically binds to the active pocket of the SARS-CoV-2 M^{pro} (Fig. 3), as apparent from higher -CDOCKER energy and -CDOCKER interaction energy. Since, simple active biomolecule like Alliin effectively binds into the active pocket of the M^{pro} under *in silico* conditions it is quite possible to design pharmacophore molecules based on the structural and functional identity of Alliin and eventually can be used in the pharmaceutical sector. Chemical synthesis of Alliin can be cost effective as compared to the isolation process from specific plants.

CONCLUSION AND FUTURE PERSPECTIVES

The emerging coronavirus has become a nightmare throughout the globe. Though many attempts were made to defeat the virus, we are incapable of targeting the stem of it. This study has focused on the use of phytochemicals for treatment. The solved crystal structure of SARS-CoV-2 i.e. main protease (M^{pro}) can be considered as the root molecule and inhibitory ligands may be screened for detection of bioactive molecules. *In silico* molecular docking revealed the effectiveness of Alliin to bind to the active site of SARS-CoV-2 main protease. The current *in silico* molecular docking based study reveals that Alliin can target the reported SARS-CoV-2 M^{pro}. It would be extremely noteworthy being confirmed *in vivo*. It is crucial to develop diagnostic tools, potential therapeutics and antibodies selectively for the COVID-19 proteins. Phytochemical like Alliin is commercially available and thus may be

effectively prescribed to circumvent the current global scenario. Essentially, this study makes an attempt to reveal simple phytochemical like Alliin which can be employed for designing novel therapeutics.

Author contribution statement

KBS and GKP conceived the idea. GKP, SBN, PKP, SKS, CR performed the experiments. KBS and GKP analyzed the data. All authors have significant contribution in drafting the manuscript.

Funding

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Conflict of interest

The authors declare that they have no conflict of interest.

REFERENCES

1. Chen N, Zhou M, Dong X, et al. 2020. Epidemiological and clinical characteristics of 99 cases of 2019 novel coronavirus pneumonia in Wuhan, China: a descriptive study. Lancet 395, 507-513.
2. Huang C, Wang Y, Li X, et al. 2020. Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China. Lancet 395, 497-506. https://doi.org/10.1016/S0140-6736(20)30183-5.
3. Lu R, Zhao X, Li J, et al. 2020. Genomic characterisation and epidemiology of 2019 novel coronavirus: implications for virus origins and receptor binding. Lancet 395, 565-574.
4. Wu F, Zhao S, Yu B, et al. 2020. A new coronavirus associated with human respiratory disease in China. Nature 579, 265-269.
5. Chan JFW, Yuan S, Kok KH, et al. 2020. A familial cluster of pneumonia associated with the 2019 novel coronavirus indicating person-to-person transmission: a study of a family cluster. Lancet 395, 514-523.
6. Li Q, Guan X, Wu P, et al. 2020. Early Transmission Dynamics in Wuhan, China, of Novel Coronavirus–Infected Pneumonia. N Engl J Med 1-9.
7. Liu W, Morse JS, Lalonde T, Xu S. 2020. Learning from the Past: Possible Urgent Prevention and Treatment Options for Severe Acute Respiratory Infections Caused by 2019-nCoV. Chem Bio Chem 730-738.
8. Wrapp D, Wang N, Corbett KS, et al. 2020. Cryo-EM structure of the 2019-nCoV spike in the prefusion conformation. Science 1263,1260-1263.
9. Lung Jrhau, Yu-Shih Lin, Yao-Hsu Yang, et al. 2020. The potential chemical structure of anti-SARS-CoV-2 RNA-dependent RNA polymerase. J Med Virol 0-1.
10. Ton A-T, Gentile F, Hsing M, et al. 2020. Rapid Identification of Potential Inhibitors of SARS- CoV-2 Main Protease by Deep Docking of 1.3 Billion Compounds. Mol Inform 1-18.
11. Dassault Systèmes BIOVIA, DISCOVERY STUDIO, San Diego: Dassault Systèmes, 2020.
12. Panigrahi Gagan Kumar, Sahoo Shraban Kumar and Satapathy Kunja Bihari. 2020. In silico Molecular Docking-Based Screening of Phytochemicals Targeted against Glypican-1. IJONS. 59(10), 18708-18712.

Table 1: -CDOCKER ENERGY and -CDOCKER INTERACTION ENERGY values generated for the interaction of Alliin with the active site of SARS-CoV-2 main protease (M^{pro}).

Ligand		Receptor		Interaction Status		
SDF accession	Phytochemical	Protein	PDB accession	Docking Result	CDOCKER ENERGY	CDOCKER INTERACTION ENERGY
CHEBI:2596	Alliin	COVID-19 Main Protease	6M03	POSITIVE	9.36	12.78

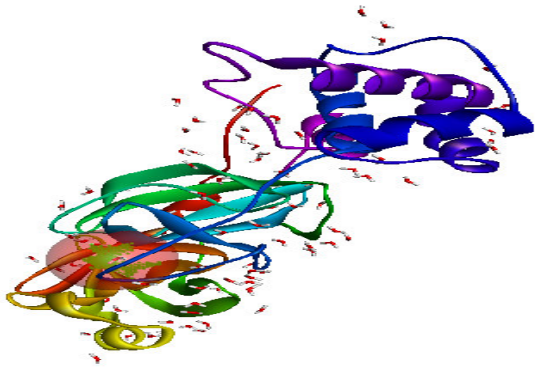

Fig. 1: 3-D Structure of the SARS-CoV-2 M^{pro} showing the active site of the protein.

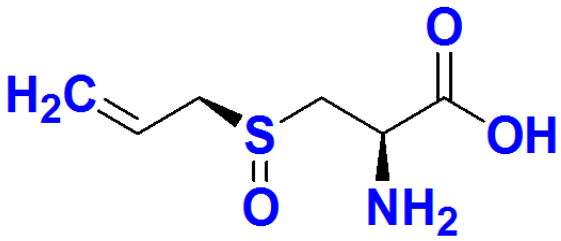

Fig. 2: Chemical structure of Alliin

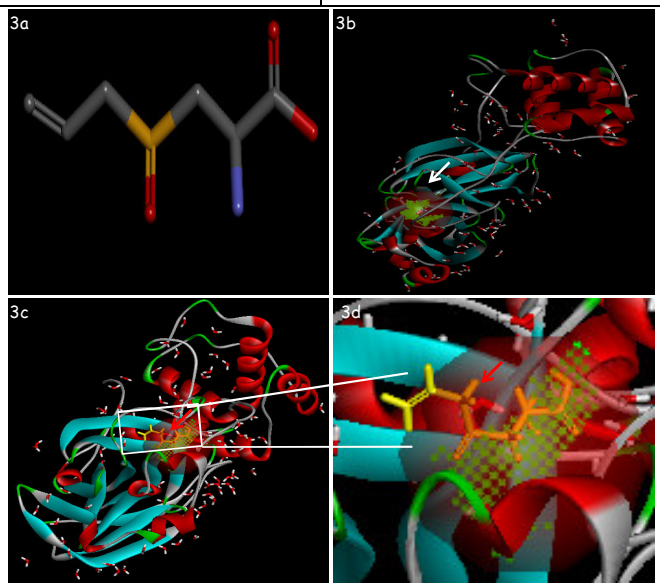

Fig. 3: The active site of the SARS-CoV-2 main protease (M^{pro}) interacts with Alliin. 3a: Phytochemical, Alliin. 3b: Free form of the M^{pro}. 3c: M^{pro} associated with the ligand, Alliin. 3d: Magnified image showing the association of the Alliin with the M^{pro}. (The white coloured arrow and the red coloured arrow indicate the active site of the M^{pro} and binding of Alliin respectively).

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RESEARCH ARTICLE

Plant Resource Used in Basanta Panchami for Worshipping Goddess Saraswati in Odisha, India

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ABSTRACT

Biodiversity, short for biological diversity is a term coined to emphasize the many complex kinds of variations that exist within the organisms and different level of organism. Biodiversity being the most precious gift of the nature is the life supporting system of the individuals. Plants are really important for the planets and all living things. We, the living beings need plants to live. We eat them and live in them. Among all the religions, Hinduism is the most widely professed faith in India and world'sthird largest religions. Different festivals like Dola Purnima, Raja, Sabitri, Saraswati Puja, Kali Puja and many more are of great significance in Hindu custom. Being a student of an educational institution, Saraswati puja is observed devoutness and whole heartedness across Odisha. Traditional, Hindu people use a large no. of flora species and flora parts for worshiping the almighty. It has been observed that a large no. of plants and plant parts are being used for worshiping goddess Saraswati. The information about the importance of flora, uses of flora and flora parts in Saraswati puja occasion were collected through the interaction with priests and some knowledgeable senior people who are engaged in such occasion. The different plant species with their botanical name, local name, family, habitat, plant parts usage and form of uses are note down. In this paper the total number of 48 species under 47 genera and 30 families were recorded during the study.

Keywords: Biodiversity, Hinduism, Religions, Saraswati, Worshiping.

INTRODUCTION

Hinduism is one of the world's oldest religions its plethora of forms and beliefs reflex the tremendous diversity of India, it is a culture, away of life and a code of behaviour and Indians use the term "Sanatana Dharma" to describe the Hindu religions (1). The importance of plants for worshiping almighty has been explained in different Vedas. Traditionally, in Hindu religion people use a large number of plant species and plant parts for worshiping different Gods and Goddesses. Many plants are associated with religious function, rituals and also in celebration of various festivals. As the plants are present all over the world this has been given an importance place in our great Hindu culture (2).

Saraswati is Hindu goddess of knowledge, music, art, wisdom and learning. Saraswati Puja also known as Basant Panchami or Shree Panchami, is one of the most popular occasion of Hindu festivals celebrated on the fifth day of the bright half of the Hindu lunisolar calendar month of Magha, which typically falls in late January or early February. Basant in Hindu means, 'Spring' and Panchami means the '5th day', hence named Basant Panchami. Basant Panchami marks the beginning of spring and start of preparation for other measure Hindu festivals like Holi and conclusion of winter. It is celebrated throughoutIndia, especially in eastern state such as west Bengal, Odisha including north east states like Tripura and Assam (3, 4). Thus, the paper present with the main intention to emphasize on the use of plants and plant parts in Saraswati puja for worshiping of the goddess Saraswati in Odisha, India.

MATERIALS AND METHODS

Study on the documentation of plants and plant parts that are used in Basant Panchami for worshiping goddess Saraswati among Hindu community. The information was collected and the data were recorded about the priority of various plants, use of plants and plant parts, for worshiping goddess Saraswati. Information were collected through discussion and communication with some well-known specialised person like priests who perform ritual works in temples and different pandals and some knowledgeable senior persons who are involved in such occasion activity (Fig.1). The botanical names of the plants are documented and identified with the help of "The Flora of Odisha and Hennies floras" (5,6). Finally, the collected specimen is submitted in the herbarium unit of Department of Botany, Centurion University of Technology and Management, Odisha, India.

RESULTS AND DISCUSSION

The present study could document 47 plant species from 30 families which are associated with the socio- culture and religious believers and are used in different areas during the time of Saraswati puja. The information regarding the utility of different plants and plant parts were collected by interacting with elderly persons and religious headmen. Data was collected by questionnaire, interviews and discussion among local headman in their local language. Most of the species used were trees 64%, followed by herbs 11%, shrubs11%, grasses 7% and climbers 7% (Fig.2). The main plant used is *Musa sapientum* L. Different types of leaves are used for decoration, flowers for garlands, fruits, seeds for preparing prasad and plant species for worshiping. The plant species of the present study are arranged alphabetically with their botanical name, local name, family, habitat, parts used and form of use are given in Table1.

CONCLUSION

The study based on religious plants and plant parts used in Saraswati puja for worshiping, shows the importance of plants in human life. This study makes us understand how community people are contributing in conserving plants and forest of their own interest to check their inherent socio-culture and religious activities. These activities of

conserving and using of plant species in the name of socio-culture and religion has significant in todays crisis of biodiversity conservation

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REFERENCES

1. Dalasingh BK, Mahalik G, Parida S. Study on the use of plants and plant parts in Durga Puja for worshipping of goddess Durga in Odisha, India. International Journal of Management Technology and Engineering. 2018; 8:2911-2918.
2. Dash S, Mandal U, Mahalik G, Parida S. Study on the plants and plants parts used in Ganesh puja for worshiping lord Ganesh in Odisha, India. International Journal of Advance Science and Technology, 2019; 28: 63-71.
3. Elizabeth D, George SW. Encyclopedia of Religious and Spiritual Development. SAGE Publications, 2005; pp 204. ISBN 978-0761928836.
4. Rajendra K. Saraswati Puja: Worshipping knowledge, education. Times of India. Archived from the original on 10 June 2018. Retrieved 19 October 2015.
5. Saxena HO, Brahmam M. The Flora of Orissa (1994-96). Vol. 1-4. Bhubaneswar: Regional Research Laboratory and Forest Development Corporation of Orissa, 1994.
6. Haines HH. The Botany of Bihar and Orissa, 6 parts, London (1921-25). Calcutta: Botanical Survey of India, 1921.

Table 1. List of the plants and plants parts used in Basanta panchami for worshiping Goddess Saraswati

FLOWERS						
Sl. no	**Botanical name**	**Local name**	**Family**	**Habitat**	**Parts used**	**Form of use**
1.	*Cascabela thevetia* (L.) Lppold	Kaniara	Apocyanaceae	Shrub	Flower	Worshiping, garlanding
2.	*Clitoria ternatea* L.	Aparajeta	Fabaceae	Climber	Flower	Worshiping, garlanding
3.	*Hibiscus rosa-sinensis* L.	Mandara	Malvaceae	Shrub	Flower	Worshiping, garlanding
4.	*Impatiens balsamina* L.	Haraguara	Balsaminaceae	Herb	Flower	Worshiping, garlanding
5.	*Jasminum multiflorum* (Burm.f.) Andrews	Bana mali	Oleaceae	Shrub	Flower	Worshiping, garlanding
6.	*Michelia champala* L.	Swarna Champa	Magnoliaceae	Tree	Flower	Worshiping, garlanding
7.	*Nyctanthes arbour-tristis* L.	Gangaseoli/Singhara hara	Oleaceae	Tree	Flower	Worshiping, garlanding
8.	*Nerium indicum* Mill.	Kaniar	Apocyanaceae	Tree	Flower	Worshiping, garlanding

9.	*Polianthes tuberose* L.	Rajanigandha	Asparagaceae	Tree	Flower	Worshiping, garlanding
10.	*Nelumbo nucifera* Gaertin.	Padma	Nelumbonaceae	Herb	Flower	Worshiping, garlanding
11.	*Nymphaea pubescens* Willd.	Dhalakain	Nymphaeceae	Herb	Flower	Worshiping, garlanding
12.	*Nymphaea nouchali* Burm.f.	Nilakain	Nymphaeceae	Herb	Flower	Worshiping, garlanding
13.	*Tagetes erecta* L.	Gendu	Asteraceae	Herb	Flower	Worshiping, garlanding
LEAVES						
1.	*Aegle marmelos* (L.) Corr.	Bela	Rutaceae	Tree	Leaves	Worshiping
2.	*Cynodon dactylon* (L.) Pers.	Duba	Poaceae	Grass	Leaves	Worshiping
3.	*Desmostachya bipinnata* (L.) stapf	Kusa	Poaceae	Grass	Leaves	Worshiping
4.	*Mangifera indica* L.	Amba	Anacardiaceae	Tree	Leaves	Worshiping
5.	*Mimusops elengi* L.	Baula	Sapotaceae	Tree	Leaves	Worshiping
6.	*Musa sapientum* L.	Kadali	Musaceae	Tree	Leaves	Decoration
7.	*Osimum sanctum* L.	Tulsi	Lamiaceae	Herb	Leaves	Worshiping
8.	*Phoenix Sylvestris* (L.) Roxb.	Khajuri	Arecaceae	Tree	Leaves	Decoration
9.	*Piper betel* L.	Pana	Piperaceae	Climber	Leaves	Worshiping
10.	*Polyalthia longifolia* (Sonn.) Thw.	Debadaru	Annonaceae	Tree	Leaves	Decoration
11.	*Shorea robusta* Gaertn.f.	Sala	Dipterocarpaceae	Tree	Leaves	Decoration
12.	*Ziziphus mauritiana* Lam.	Barakoli	Rhamnaceae	Tree	Leaves	Worshipping
FRUITS						
1.	*Anacardium occidentale* L.	Kaju	Anacardiaceae	Tree	Fruits	Used in prasad
2.	*Ananas comosus* (L.). Merr.	Sapuri	Bromeliaceae	Shrub	Fruits	Used in prasad
3.	*Annona squamosa* L.	Ata	Annonaceae	Tree	Fruits	Used in prasad
4.	*Citrus reticulata* Blanco	Kamala	Rutaceae	Tree	Fruits	Used in prasad
5.	*Cocos nucifera* L.	Ndia	Arecaceae	Tree	Fruits	Used in prasad
6.	*Cucumis sativus L.*	Kakudi	Cucurbitaceae	Climber	Fruits	Used in prasad
7.	*Musa sapintum* L.	Kadali	Musaceae	Tree	Fruits	Used in prasad
8.	*Phoenix Sylvestris* L.	Khajuri	Arecaceae	Tree	Fruits	Used in prasad
9.	*Psidium guajava* L.	Pijuli	Myrtaceae	Tree	Fruits	Used in prasad
10.	*Punica granatum* L.	Dalimba	Punicaceae	Tree	Fruits	Used in prasad
11.	*Pyrus communis* L.	Naspati	Rosaceae	Tree	Fruits	Used in prasad
12.	*Pyrus malus* L.	Seu	Rosaceae	Tree	Fruits	Used in prasad
13.	*Terminalia chebula* Retz.	Harida	Combretaceae	Tree	Fruits	Used in prasad
14.	*Terminalia bellirica* (Gaertn.) Roxb.	Bahada	Combretaceae	Tree	Fruits	Used in prasad
15.	*Vitis vinifera* L.	Angura	Vitaceae	Climber	Fruit	Used in prasad
SEEDS						
1.	*Areca catechu* L.	Gua	Arecaceae	Tree	Seeds	Worshiping
2.	*Brassica napus* L.	Sorisha	Brassicaceae	Shrub	Seeds	Worshiping
3.	*Elettaria cardamomum* L.	Gujarati	Zingiberaceae	Tree	Seeds	Used in prasad
4.	*Oryza sativa* L.	Dhana	Poaceae	Grass	Seeds	Worshiping

5.	*Piper nigrum* L.	Golamaricha	Piperaceae	Shrub	Seeds	Used in prasad
6.	Syzygium aromaticum (L.) Merrill & Perry	Labanga	Myrtaceae	Tree	Seeds	Used in prasad
7.	Vigna radiate (L.) R. Wilczek	Muga	Fabaceae	Herb	Seeds	Used in prasad
WOODS						
1.	*Mangifera indica* L.	Amba	Anacardiaceae	Tree	Wood	Worshiping
2.	*Santalum album* L.	Shweta Chandana	Santalaceae	Tree	Wood	Worshiping
3.	*Shora robusta* Gaertn.f.	Sala	Dipterocarpaceae	Tree	Wood	Worshiping
OTHERS						
1.	*Cocos nucifera* L.	Nadia	Arecaceae	Tree	Fibre	Worshiping
2.	*Saccarum officinarum* L.	Akhu	Poaceae	Grass	Stem	Worshiping
3.	*Shora robusta* Gaertn.f.	Sala	Dipterocarpaceae	Tree	Wax (Jhuna)	Worshiping

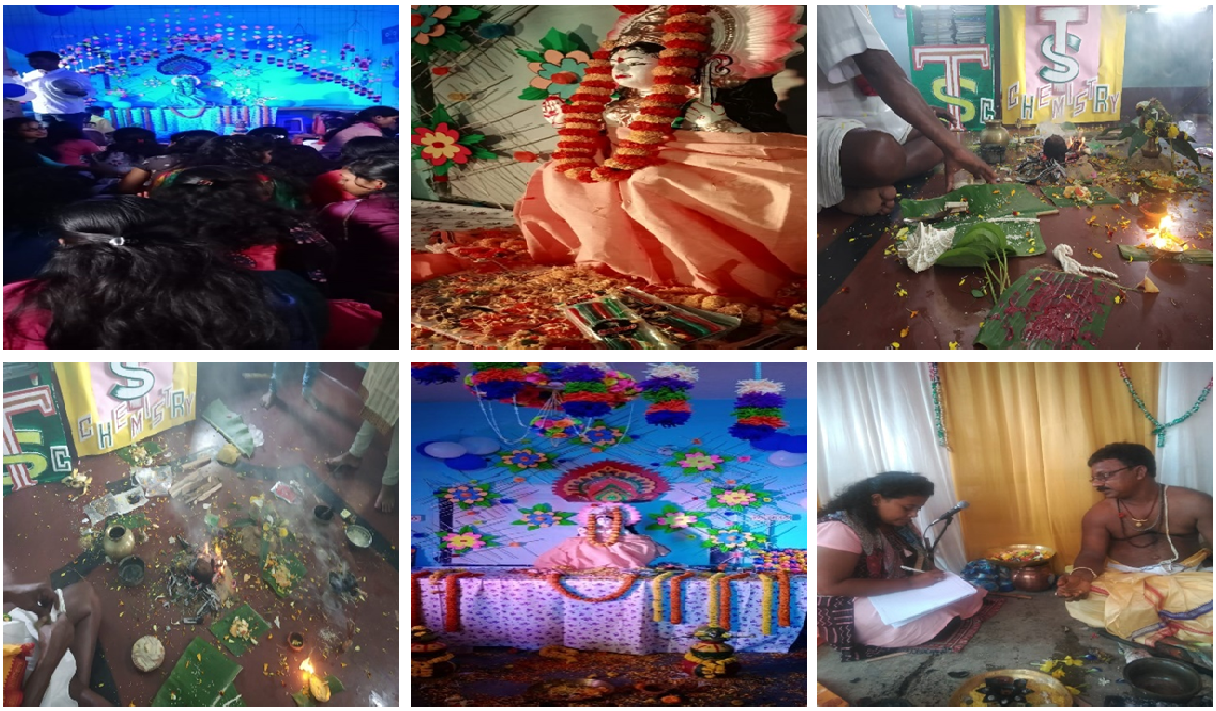

Fig.1. Data collected through the survey and interaction with the priests

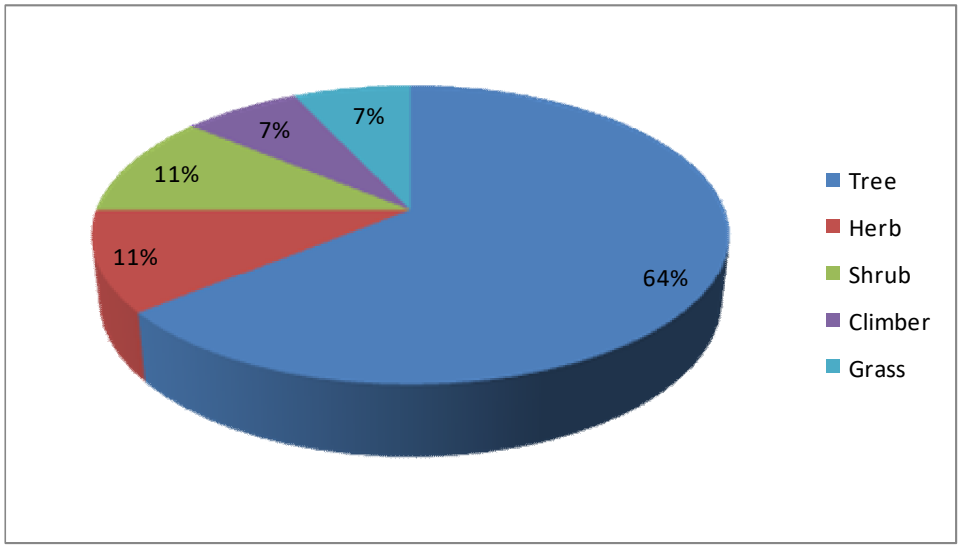

Fig. 2. Habit wise distribution of the plant species

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RESEARCH ARTICLE

Wild Native Oil Yielding Plants and Their Utilization by the Tribals of Nabarangpur District of Odisha, India

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ABSTRACT

Seed is the fundamental and essential contribution for effective yield generation, which holds the way to the ranch efficiency and benefit. Oils obtained are either used for edible purposes or are found to be used as medicinal uses and cooking purposes. Recently oil yielding plants attract more attention due to an increasing demand for their vegetable oils, live stock feeds, pharmaceutical biofuels and other chemical industries. Based on extensive and intensive explorations and observations the diversity and performance studies of native oil yielding important plants were studied in four blocks of Nabarangpur such as Papadahandi, Dabugaon, Umerkote and Raighar respectively. A total of 24 oil yielding natively growing plant species belonging to 17 families were documented. These oil yielding plants were used by the different local people and tribals of Nabarangpur. Among them, *Brassica* species (Mustard) and *Sesamum indicum* L. (Rasi) is the major oil seed crop which covers the area of about 233 hectares in four blocks of Nabarangpur. The oil seed cultivation practices along with the climatic conditions prevailed in these particular area has its impact on yield of oil seeds. Good cultivation practices are needed to preserve and for getting maximum yield which can be used as alternatives for their livelihood.

Keywords: Biofuels; Cultivation; Nabarangpur; Oils; Pharmaceutical.

INTRODUCTION

India has been recognized as one of the world with mega diversity. Man has depended on plants ever since life began. Human wellbeing relies upon the nature of the earth in which individuals live (1). The interrelationships among society and nature, and the significance of environment to human health rely upon biodiversity which have

direct effect on human-prosperity too. Regardless of the essential dependence of horticultural social orders on domesticated plants and animals for sustenance, the convention of consuming wild plants has not been totally eradicated. A large number of individuals, especially tribals and rural communities in many nations still gather and consumed a wide assortment of wild plant and plant products to meet their nourishment necessities (2, 3).

Oilseeds are among the significant cash crops of India. For plants, they are imperative as reserves of energy to maintain the germination of the seed; for human these are considered as proficient food sources of energy. The synthetic compositions of seeds of cultivated and wild species are more thoroughly known since these comprise a large share of the food supply and industrial raw materials. Information on the seeds of wild species is relatively scanty. However, the search for new sources as industrial raw materials is gradually providing more and more information about seeds of wild plants. Seed chemistry is an interesting subject for scientific study with the result that much information about both cultivated and wild species is being accumulated (4). The present study was aimed to document the availability, consumption and management of oil yield plants and their uses by the tribals of Nabarangpure district of Odisha.

MATERIALS AND METHODS

Study area

Nabarangpur District, also known as Nabarangapur District and Nawarangpur District, is a district of Odisha, India. The study was conducted in the Nawarangpur district of the Odisha state of India during the year 2018-2019. The city of Nabarangpur is the district headquarters. Most of its population is tribal, and most of the land is forested. Situated in the southwest corner of Odisha, it borders Koraput District. Nabarangpur district is situated at 19.14' latitude and 82.32' longitude at an average elevation of 1,876 feet (572 m) (Fig. 1).

Field Survey

Various tribal rich forest pockets of the district were identified and field trips were conducted at regular intervals in differed seasons. Tribal uses of plants and oil seeds were studied *in situ* by establishing close intimacy with the tribals. Care was taken to prioritize vulnerable areas for immediate attention especially forest pockets which are under intensive mining activity. Folklore claims were documented along with voucher specimens (5).

Plant and oil seed Collection and Herbarium Studies

The supportive plants and oil seeds were collected, processed, critically studied, identified and preserved in the Herbarium and seeds were deposited in Department of Botany, School of Applied Sciences, Centurion University of Technology and Management, Odisha. Voucher specimens were identified by referring standard local floras (6).

Local Names

Vernacular names in vogue in the different tribal languages and Odia were given.

RESULT AND DISCUSSION

The results of the oil yielding plants survey are presented in table 1. A total of 24 plants species belonging to 17 families were documented. For each species the following information was provided: Botanical name, family, local name, habit/habitation/ domestication, parts used, rank of uses and abundance. Among family Fabaceae were more dominate followed by Anacardiceae, Brassicaceae and Euphorbiaceae (Fig. 2). Habit wise analysis of available species indicated that 13 (54%) were trees followed by 6 (25%) herb, 4 (17%) shrub and 1 (4%) climber (Fig. 3). Comparison of the plant parts used as an oil yielding source indicates that the seeds predominate followed by stem, leaf and flower (fig. 4).

CONCLUSION

The oil yielding crops have been the foundation of farming economy in perspective on its commercial as well as utilization esteem. Oil yielding plants have been used as cooking oil, other food supplements and other uses. The finding of this study provided that, most of the plants used by the community of study area oil yield substances in seed, stem, flower and leaf parts of surveyed plants. Studies have also shown that oils from unconventional native sources will not only fill the gap between demand and supply, it could be a source of earning of the foreign exchange. It is believed that the oil bearing plant resource of the Nabarangpure area provides a checklist of the floristic diversity which will serve as a prepared reference for scientific research.

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Author's Contribution

GM and HN: Conceptualized and designed the research work; HN: Survey, collected and documented field data; and GM and HN: All authors prepared the manuscript.

Competing Interest

Authors do not have any conflict of interest to declare

REFERENCES

1. Food and Agriculture Organization of the United Nations (FAO), Annual Report: The state of food insecurity in the world, Food and Agriculture Organization of the United Nations Viale delle Terme di Caracalla, Rome, Italy; 2004.
2. Balemie K, Kebebew F. Ethnobotanical study of wild edible plants in Derashe and Kucha Districts, South Ethiopia. J Ethnobiol Ethnomed. 2006; 2:53-61.
3. https://link.springer.com/article/10.1186/1746-4269-2-53
4. Bharucha Z, Pretty J. The roles and values of wild foods in agricultural systems. Philosophical Transactions of the Royal Society B. Biolog Sci. 2010; 365**:** 2913-2926. https://doi.org/10.1098/rstb.2010.0123
5. Naiman MO, Chaudhary AR, Banerji R, Nigam SK. Oilseeds and their Utilization, Editors Suri RK and Mathur KC., Rohini Publishing House, Dehradun (India); 1984.
6. Mahalik G, Satapathy KB, Sahoo S. Ethnobotanical survey of plants used in treatment of urinary disorders in Dhenkanal district of Odisha, India. J Environ Sci, Toxico and Food Tech. 2015; 9(8): 58-63. DOI: 10.9790/2402-09815863
7. Saxena HO, Brahmam M. The Flora of Orissa, Vol. 1- 4. Regional Laboratory and Forest Development Corporation of Orissa, Bhubaneswar (1994-1996); 1994.

Table 1. List of oil yielding plant species in Nabarangpur district of Odisha, India

Sl. No.	Botanical Name	Family	Local name	Habit/ Habitat/ Domestication	Parts used	Rank of use	Abundance
1	*Anacardium occidentale* L.	Anacardiaceae	Kajubadam	Tree , Cultivated	Seed	+	Common
2	*Arachis hypogaea* L.	Fabaceae	Chinabadam	Herb , Cultivated	Seed	+	Occasional
3	*Azadirachta indica* A. Juss.	Meliaceae	Neemba, Limb	Tree , Wild	Seed , Leaf , Stem	++	Common
4	*Brassica nigra* (L.) W.D.J. Koch	Brassicaceae	Kala sorisa	Herb Cultivated	Seed	+++	Common
5	*Brassica juncia* (L.) Czern.	Brassicaceae	Dhala sorisa	Herb, cultivated	Seed	+++	Common
6	*Cocos nucifera* L.	Arecaceae	Nadia	Tree Caudex Cultivated	Seed , Leaf	++	Common
7	*Eucalyptus globulus* Labill.	Myrtaceae	Nilagiri	Tree, Wild	Seed, Stem	+	Rare
8	*Glycine max* (L.) Merr.	Fabaceae	Soyabean	Climbers , Cultivated	Seed	++	Rare
9	*Gossypium arboretum* L.	Malvaceae	Tula	Herb, cultivated	Seed	+	Common
10	*Helianthus annuus* L.	Asteraceae	Suryamukhi	Shrub , Cultivated	Seed	++	Common
11	*Jatropha curcas* L.	Euphorbiaceae	Dumajoda, Bhendra	Shrub , Cultivated	Seed	+	Rare
12	*Linum usitatissimum* L.	Linaceae	Pesi	Herb Cultivated	Seed	+++	Occasional
13	*Madhuca longifolia* (Roxb.) A. Chev.	Sapotaceae	Mahula, Tolgachh	Tree , Wild	Seed, Stem, Flower	+++	Common
14	*Martynia annua* L.	Martyniaceae	Baghanauhi	Shrub , Wild	Seed	++	Rare
15	*Millettia pinnata* (L.) Panigrahi	Fabaceae	Karanja	Tree , Wild	Seed , Stem	+++	Common
16	*Phyllanthus emblica* L.	Phyllanthaceae	Aonla	Tree , Wild	Seed, Stem	+	Occasional

17	*Ricinus communis* L.	Euphorbiaceae	Joda	Shrub Cultivated/ Wild	Seed	++	Common
18	*Schleichera oleosa* (Lour.) Oken	Sapindaciae	Kusuma	Tree , Wild	Seed, Stem	+++	Common
19	*Sesamum indicum* L.	Pedaliaceae	Rasi	Herb , Cultivated	Seed	+++	Common
20	*Semecarpus anacardium* L.f.	Anacardiaceae	Bhaliya	Tree, Wild	Seed	++	Occasional
21	*Senna Tora* (L.) Roxb.	Fabaceae	Chakunda	Tree , Wild	Seed	+	Rare
22	*Shorea robusta* Gaertn.	Dipterocarpaceae	Sal, Sarjam, Saragi	Tree , Wild	Seed , Stem	++	Occasional
23	*Strychnos nux-vomica* L.	Loganiaceae	Kochila	Tree, Wild	Seed	++	Occasional
24	*Syzygium aromaticum* (L.) Merrill & Perry	Myrtaceae	Lobonga	Tree, Cultivated	Flower bud, Stem	++	Rare

Fig.1. Map of the study area

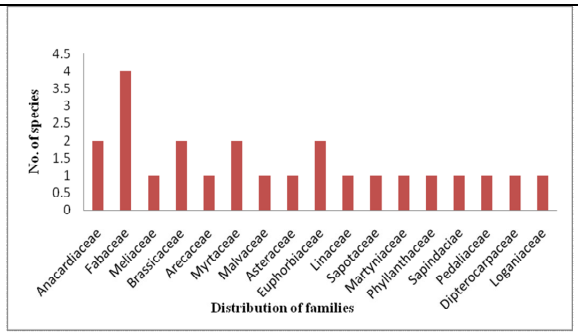

Fig. 2. Family wise distribution of plant species

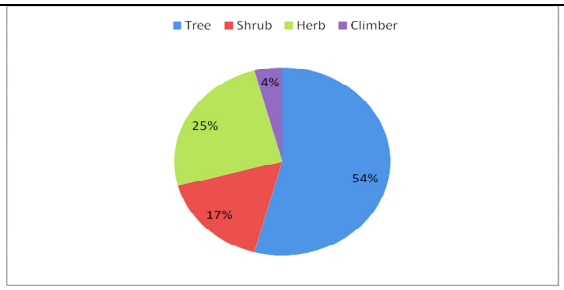

Fig. 3. Habit-wise distribution of plant species (%)

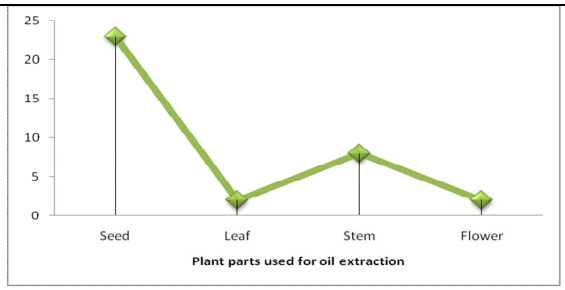

Fig.4. Different plant parts used for oil extraction

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RESEARCH ARTICLE

Comparative Study of the Effect of Organic Fertilizer and Chemical Fertilizer on Brinjal Plant (*Solanum melongena* L.)

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ABSTRACT

Decades back, agrochemicals were presented going for improving harvest yields and at protecting crops from pests. Nowadays agrochemical has come to be crucial to modern-day agriculture to feed the growing population. Heavy metals such as lead, chromium, arsenic, zinc, cadmium, copper and nickel are accumulated in the plants. Heavy metal contamination in soils and in the plants is a major environmental concern that affects large areas worldwide as well as human health. The present research is comparison between accumulation of heavy metals in *Solanum melangena* L. by use of different organic and chemical fertilizer used in Dharmasala area of Jajpur district of Odisha and to know the adverse effect agrochemicals on the plants. Preliminarily plantation of *Solanum melongena* was done on two fields using organic and chemical fertilizer respectively. The chemical fertilizer is NPK and pesticide is *Chlorpyrifos* and the organic fertilizer used was a mixer of cow dung, vegetable peels, dead plant organic matters and combination of organic and inorganic matters. Samples of fruits of *Solanum melongena* was collected two different fields. Heavy metal analysis was done using X-ray fluorescence spectroscopy. These agrochemicals cause accumulation of different heavy metals in the soil like zinc and copper, which can also accumulate in the plants out of which some are very much carcinogenic and cause health disorders. From this paper we conclude that chemical fertilizer increase yield but also harm the environment and the long-term uses can be catastrophic. So beside used of chemical product we can use biological products for good health and better environment

Keywords: Agrochemical, Fertilizer, Heavy metals, Hormones, *Solanum melongena*

INTRODUCTION

Organic and inorganic fertilizers are important for plant growth. Each fertilizer provides plants with the nutrients required for optimum performance. Organic fertilizers are used for several centuries whereas chemically synthesized inorganic fertilizers were only widely developed during the industrial revolution. Inorganic fertilizer has significantly supported global increase, it's been estimated that nearly half the people of the world are currently fed as a results of artificial nitrogen fertilizer use (1). Commercial and farming has been and remains relying on the utilization of inorganic fertilizers for growing crops, this is often because they are easy to use, quickly absorbed and utilized by crops (2). The effect of organic and NPK are studied on the nutritional quality of Amaranthus. Hussain et al., (2013) (3) reported that organic material alone or together with NPK significantly increased CP, ash and EE while CF was reduced. The NKP gave least values of CP, CF ash and EE compared with organic material.

Organic material alone or integrated with NPK increased nutritive quality. Yoldas et al., (2011) (4) studied the effect of organic and inorganic fertilizers on yield and mineral content of onion and reported within the year, that treatments influenced K content, but didn't influence N, P, Ca, Na, Mg, Fe, Zn, Cu and Mn contents of the onion bulb. In the second year, the treatments influenced Na content, but failed to influence the others. Coolong et al., (2004) (5) reported that N, P, Mn, Fe and Zn content of bulb were increased by N treatments but the content of N was decreased by N doses. Potassium, Cu and Mo contents were not suffering from the treatments. *Solanum melongena* is commonly referred to as the Brinjal or Egg plant. Eggplant is a plant species belongd to family Solanaceae. *Solanum melongena* is grown international for its suitable for eating fruit. The present study evaluates the soil contamination and bioaccumulation of six heavy metals Rubidium (Rb), Tin (Sn), iron (Fe), copper (Cu), Silicon (Si), and potassium (K) as well as two types of fertilizers, organic and inorganic on Egg plant (6).

MATERIALS AND METHODS

Study area

Jajpur is one among the main agriculture districts of the state. it is surrounded by hills, rivers and forest. It's constituted by two no's of agricultural zone, three no's of agriculture districts and 10 no's of blocks out of 1,42,750 hector of cultivated land, 1,11,100 hector is paddy land during Kharif season. The fertile loamy soil of the district is help full for increase of the crop productivity. Within the district soils like Loamy, sandy, clayey and red also are seen. Rapid increase of industrialization within the state and also within the district is decreasing the fertile farmland. Brinjal is the main crop whereas Groundnut, Mung, Biri, Vegetable and Sugarcane are grown mainly in Rabi season. Jajpur district is known for brinjal cultivation within the state. Normaly Brinjal is cultivated in 30,000 to 35,000 hector within the district. Additionally the state is proud for cultivation of vegetables in Dharmasala, Rasulpur, Barachana and Jajpur blocks of the district (7)

Fertilizer treatment

Two type's fertilizer treatments were applied: the first treatment is organic fertilizer (OF) and the second fertilizer is chemically synthesized NPK fertilizer (8).

Soil preparation and planting

First, the experimental area was tilled and then parcels were created. Then the fertilizers applied according to the experiment plan. After that, the drip irrigation system was established (Fig. 1). The egg plant seedlings were planted according to the experiment plan, the spacing between rows was 90 cm, the spacing within rows is 50 cm, each parcel contains 6 rows, in each row 20 plants and each plot contains 1400 plants (8).

XRF analysis

The fruit sample were dried, homogenized and sieved at 250 µm particles sizes. XRF analyzes were carried out Advanced Testing and Calibration laboratory in Centurion University Of Technology& Management using a handheld Epsilon 1 Pan analytical XRF spectrometer. By automatically adjusting for matrix effect, epsilon 1 Pan analytical XRF spectrometer analyzers are able to determine the content of soil sample typically in seconds, without any requirement for instrument user to input empirical, sample specific calibrations (Fig.1). The sample name, spectrum& element composition are stored in a dedicated library (9).

RESULTS AND DISCUSSION

The present study observed that the application of five parameters i.e. T_1, T_2, T_3 , T_4 , T_5 (Cow dung, Vegetable peels, dead plant matters, chemical fertilizer and mixture of organic and inorganic matters) Solely or combined application had a great influence at all the stages of the bringal crop. Significant differences were observed in all parameters like number of branches, length of fruit, number of fruit, plant height and fruit weight. Highest plant heights (95.34 cm) were observed in T_5 followed by T_4 (82.56 cm), T_3 (72.7 cm), T_2 (60.41cm), T_1(58.2cm) (Table 1). The highest number of branches per plant (21 nos.) was recorded in T_5 followed by T_3 (18 nos.), T_4 (17 nos.), T_2 (16nos.), T_1 (14 nos.). If we compare length of fruits, 15.3 cm of length was measured in combination of organic and in inorganic fertilizer (T_5) followed by 14.9 cm (T_4), 12.7 cm(T_3), 10.4 cm (T_2), 10.1 cm (T_1). The data on fruit weight 75 gm in T_5 highest as influenced by the combination of organic and inorganic fertilizers at the all the stages. In all the treatments the number of fruits were very less in T_1 i.e 9 fruits/ plant, but highest number were recorded in T5 i.e. 14 fruits/ plant.

Combination of organic and inorganic fertilizer)

Comparable outcomes were accounted for by Naidu et al., (1999) (10) revealed that the morphological parameters were influenced altogether because of the utilization of various blend of organics, chemicals, biofertilizers. Satya Vani (2014) (11) portrayed that mycorrhizal spore populace in rhizosphere soil just as the level of mycorrhizal contamination in plant roots varied with the progressions in physico-chemical variables of the soils of brinjal.

XRF analysis

In XRF data analysis it is found that chemical fertilizer has some heavy metal like Cu (0.231%) followed by Zn (0.193%). The range of Cu in fruits were (0.231%) and Zn (0.193%). In organic fertilizer K is highest 79.032% followed by Cl, P, S, Si, Eu, Sn, Rb and Fe i.e 7.420, 4.519, 2.912, 1.631, 1.527, 0.570, 0.218 and 0.046 (Table-1). Similarly Islam and Hoque (2014) (12) also reported that the concentration of Cu in brinjal range from 13.57–19.90 mg/kg while Zhu et al. (2011) (13) reported that the concentrations of copper 0.214–0.875 (µg/g) in brinjal. In another observation of Islam and Hoque (2014) (12) also found that the concentration of Pb in brinjal range from 0.06–3.5 mg/kg while Alamgir and Chakarabarty (2000) (14) also showed the range of Pb 10.04 mg/kg for the vegetable cultivation in Bangladesh condition.

CONCLUSION

From the above result, it may be concluded that in *Solanum melangena* production application of organic fertilizer source of nutrients can be more productive and this will also sustain the fertility and productivity of soil. But the use of chemical fertilizer may harm soil micro-flora as well as human health. From this we concluded that agrochemicals increase yield, but also harm the environment and the long-term uses can be catastrophic. So beside used on chemical product we can use organic fertilizer products for good health and a better environment.

REFERENCES

1. Erisman JW, Sutton MA, Galloway J, Klimont Z, Winiwarter W. How a century of ammonia synthesis changed the world. Nature Geoscience. 2008; 1(10): 636-639.
2. Masarirambi MT, Hlawe MM, Oseni OT, Sibiya TE. Effects of organic fertilizers on growth, yield, quality and sensory evaluation of red lettuce (*Lactuca sativa* L.)'Veneza Roxa'. Agriculture and Biology Journal of North America. 2010; 1(6):1319-1324.
3. Hussain A, Alamzeb S, Begum S. Accumulation of heavy metals in edible parts of vegetables irrigated with waste water and their daily intake to adults and children, District Mardan, Pakistan. Food chemistry. 2013; 136(3-4):1515-1523.
4. Yoldas F, Ceylan S, Mordogan N, Esetlili BC. Effect of organic and inorganic fertilizers on yield and mineral content of onion (*Allium cepa* L.). African Journal of Biotechnology. 2011; 10(55):114488-114482.
5. Coolong TW, Kopsell DA, Kopsell DE, Randle WM. Nitrogen and sulfur influence nutrient usage and accumulation in onion. Journal of plant Nutrition. 2005;27(9):1667-1686.
6. Youssef MA, El-Gawad AM. Accumulation and translocation of heavy metals in eggplant (*Solanum melongena* L.) grown in a contaminated soil. Journal of Energy, Environmental & Chemical Engineering. 2018; 3(1):9-18.
7. Village and Panchayats- India. Jajpur District:Odisha. 20 March 2018. Retrieved 21 June 2019.
8. Al Ali M, Gençoğlan C, Gençoğlan S. The Effects of Organic and Inorganic Fertilizer Applications on Yield and Plant Vegetative Growth of Eggplant (*Solanum melongena* L.). International Journal of Plant & Soil Science. 2019; 1-9.
9. Ene A, Bosneaga A, Georgescu L. Determination of heavy metals in soils using XRF technique. Romanian Journal of Physics. 2010; 55(7-8):815-820.
10. Naidu AK, Kushwah SS, Diwivedi YC. Performance of organic manures, bio and chemical fertilizers and their combination on microbial population of soil and growth of okra. Jawaharlal Nehru Krishi Vishwa Vidhyalaya Research Journal. 1999; 33(1-2):34-38.
11. Vani MS, Hindumathi A, Bhumi NR. Arbuscular mycorrhizal fungi associated with rhizosphere soils of brinjal cultivated in Andhra Pradesh, India. International Journal of Current Microbiology and Applied Sciences. 2014; 3(5):519-529.
12. Islam MS, Hoque MF. Concentrations of heavy metals in vegetables around the industrial area of Dhaka city, Bangladesh and health risk assessment. International Food Research Journal. 2014 ;21(6): 2121–2126.
13. Zhu F, Fan W, Wang QL, Yao S. (2011). Health risk assessment of eight heavy metals in nine varieties of edible vegetable oils consumed in China. Food and Chemical Toxicology. 2011; 49:3081–3085.
14. Alamgir M, Chakarabarty KL (2000). Cadmium and lead contents in edible vegetable of Bangladesh. Bangladesh Journal of Science and Technology. 2000; 2(1):75-86

Table 1. Effect of organic and chemical fertilizer on growth and yield characters of *Solanum melangena* L.

Treatment	No. of Branches	Length of fruit (Cm)	No. of Fruits /plant	Plant height (cm)	Fruits weight (gm)
T_1	14	10.1	9	58.2	27
T_2	16	10.4	11	60.41	34
T_3	18	12.7	12	72.7	51
T_4	17	14.9	12	82.56	70
T_5	21	15.3	14	95.34	75

***(T_1- Cow dung, T_2- Vegetable peels ,T_3- Dead plant organic matters , T_4- Chemical fertilizer , T_5-**

Table 2. Concentration of different elements present in *Solanum melangena* L. fruit

Organic fertilizer										
Elements	Si	P	S	Cl	K	Mn	Fe	Rb	Sn	Eu
Conc. (%)	1.631	4.519	2.912	7.420	79.032	0.125	0.046	0.218	0.570	1.527

Chemical Fertilizer											
Elements	Si	P	S	Cl	K	Fe	Cu	Zn	Rb	Sn	Eu	Re
Conc. (%)	1.221	4.209	3.195	7.126	79.348	2.412	0.231	0.193	0.230	0.621	1.175	0.039

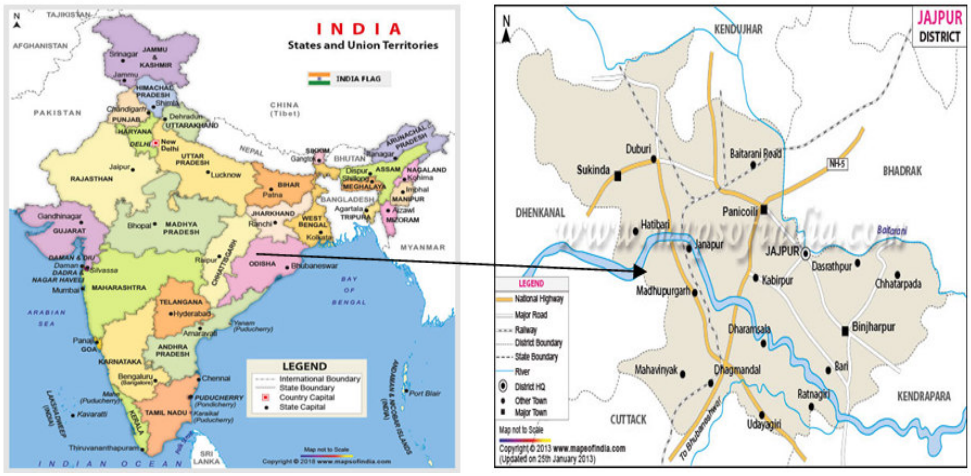

Fig.1. Map of study area

Fig. 2. During Field and lab work

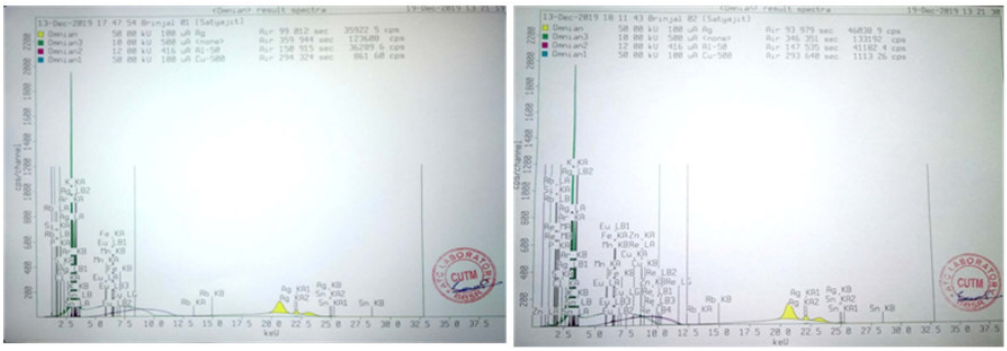

Fig.3 XRF data of *Solanam melangena* (Fruit)
A.Organic fertilizer B. Chemical fertilizer

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RESEARCH ARTICLE

Efficacy of *Nyctanthus arbour-tristis, Phyllanthus amarus* and *Cymbopogon citratus* used in the Traditional Treatment of Typhoid against *Salmonella typhimurium*

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ABSTRACT

Abstract- Medicinal plants are geared toward the development of new antibiotics and the use of medicinal plants in the treatment of typhoid fever. Typhoid fever is a bacterial infection caused by *Salmonella* species namely, *Salmonella typhimurium*. The threat to human health posed by multidrug-resistant strains of *Salmonella typhimurium* is of growing concern. Generally, there has been increasing resistance and multidrug resistance to almost all classes of antibiotics. This has rendered treatment with antibiotics difficult and costly. The present study was undertaken to document how typhoid is naturally treated. The antibacterial potential of three medicinal plants viz. *Nyctanthes arbour-tristis* L., *Phyllanthus amarus* Schumach. & Thonn., and *Cymbopogon citratus* (Dc.) Stapf were evaluated on *S. typhimurium*. The crude leaf extracts prepared in ethanol were used to assess their antibacterial potential in terms of zone of inhibition of bacterial growth, which was tested by the agar well diffusion method. Ethanol extracts of plant parts have shown significant antibacterial activity against *S. typhimurium*. The highest zone of inhibition (25 mm) was obtained from *N. arbour-tristis* at concentrations 1.0 mg/ml. *C. citratus* showed a zone of inhibition 19 mm at a concentration of 1.0 mg/ml. *P. amarus* showed zone of inhibition 15 mm, 13 mm at concentration 1.0 mg/ml, 0.5mg/ml respectively. The finding supported the use of these plants for the treatment of typhoid fever.

Keywords: Antibacterial, Antibiotics, Ethanol, Medicinal, *Salmonella typhimurium*.

INTRODUCTION

In prehistoric ages, the primitive man started learning many lessons from the nature in the art of healing by combine instinct with his dissolution. His dependence and observations on the nature coupled with providence use of plant products led to the initial knowledge about economic and curative properties of plants. He explored his natural surroundings and tried many plants found around him to treat his disorder. In recent years, traditional knowledge on medicine has drawn importance all over the world. Today, plants are not only used in health care, but for best hope of source for future medicines. Traditional plant medicine still play significant role in the drug industries due to minor side effects as well as the synergetic action of the combination of compounds (1). In the improvement of human culture therapeutic plants have assumed a fundamental job, for instance religions and various functions (2). Among the assortment of present day medications, a considerable lot of them are created by implication from therapeutic plants, similar to anti-inflammatory medicine. Restorative plants are wellspring of new medications and present day meds are created in a roundabout way from plants. Curative properties of the plant are due to the secondary metabolites or the bioactive compound which fight against the various type of disorder (3).

Typhoid fever is the most precarious illness caused by the bacterium *Salmonella typhimurium*. It can be also caused by *Salmonella paratyphi*, a related bacterium which usually leads to a less severe illness. The bacteria enters in to human body through food and water and also deposited in water and food by a human carrier and are then infect other people in the area. In industrial countries it is a rare disease but in developing countries it is the most significant public health issue (4, 5). From literature and review it was found to be *S. typhimurium* is deadly sensitive to these three medicinal plants that are *Nyctanthes arbour-tristis, Phyllanthus amarus* and *Cymbopogon citrates*.

MATERIALS AND METHODS

Plant material collection

Disease free fresh leaves of *Nyctanthus arbour-tristis, Phyllanthus amarus* and *Cymbopogon citratus* were collected from the district of Kendrapara, Odisha. The plants was identified and authenticated by following "Flora of Orissa" (6).

Sample and extract preparation

Freshly collected leaf samples were washed and air-dried under shade at room temperature for 7-10 days. After drying, the samples were chopped into small pieces, and the materials were grounded into powder form using mortar and pestle. Powdered samples were then stored in air tight containers for further use (7).

Extraction of plant materials

The crude extracts of collected plant samples were weighed. 15gm of *Nyctanthus arbour-tristis, Phyllanthus amarus,* and *Cymbopogon citratus* sample were taken. The three weighed plant samples were submerged in 130 ml of ethanol for 24 hrs at room temperature at dark condition. The mixtures were filtered by filter paper then collected and stored in three centrifuge tubes.

Bacterial strain

One bacterial strain was used in this study, which is Gram negative bacteria i.e *Salmonella typhimurium* (MTCC No.3224). The bacterial strains were collected from IMTECH Chandigarh. The bacterial Strain was cultures in nutrient agar medium and incubated at 37°C for 24hrs .

Antibacterial assay

A standardized concentration of inoculum with fixed volume is spread evenly on the surface of gelled agar plate. A hole of about 6 mm in diameter is punched with a sterile cork borer aseptically in plates. A fixed volume of plant

extract was then introduced into the bored agar well and incubated at optimum temperature (bacteria - 37°C for 24 hr) depending on the test microorganism (8).

RESULTS AND DISCUSSION

The present study revealed that the tested medicinal plants *Nyctanthus arbour-tristis, Phyllanthu samarus,* and *Cymbopogon citratus* possess potent antibacterial activity against bacterial strain, which is gram negative (*salmonella typhimurium*). Ethanol extract of *p. amarus* showed activity at two tested concentration against bacterial strain (*S. typhimurium*) was 1.0mg/ml and 0.5mg/ml. The activity was observed at concentration 1.0mg/ml was 15mm, where as the activity was observed at concentration 0.5mg/ml was 13mm. Ethanolic extract of *N. arbour-tristis* showed potent activity at two tested concentration against *S. typhimurium* in 1.0mg/ml and 0.5mg/ml. It showed the activity at 1.0mg/ml was 25mm, while no activity showed at concentration 0.5mg/ml. Ethanol extract of *C. citratus* showed activity at two concentrations against *S. typhimurium* was 1.0 mg/ml and 0.5 mg/ml. The activity was observed at concentration of 1.0mg/ml was 19mm, while no activity showed at concentration 0.5 mg/ml (Fig.1). The result suggested that the ethanolic leaf extracts of *N. arbor-tristis* showed better result against *S. typhimurium* viz. 25 mm zones of inhibition as compared to *P.amarus* and *C.* citrates (Table 1).

The movement of plants separates against microscopic organisms have been read for a considerable length of time, however in progressively heightened route during the most recent three decades. During this period, various antimicrobial screening assessments have been distributed dependent on the customary Chinese, African, and Asian employments of plant based medication (9). In the current examination, the consequences of antibacterial property of three plants extracts tried against *Salmonella typhimurium* varied depending on concentrations as previously reported by (10). All tested three plants samples showed inhibition diameter against *S. typhi*, it proves that active compounds present in sufficient quantities in the extract which shows the activity with dose levels employed (11). Lack of activity can be proven by using large dose (12).

It was seen that *N. arbor-tristis* demonstrating the antibacterial action with the zone of hindrance of 25 mm against *S. typhimurium*. This could presumably have been because of the way that the pace of dynamic fixings or constituents in the plant material is higher contrasted with different plants utilized in this exploration (13).The thing that *S. tyhimurium* was more dispose to the extract of *Nyctanthus arbour-tristis* indicated the potency of this plant against typhoid.

CONCLUSION

As our lifestyle is now getting techno-savvy, we are moving away from nature, which can create a serious threat to both environment and human life leading to various diseases like typhoid etc. So to fight against this situation the ultimate method without side effect is to accept the nature as God's gift and adopting herbal medicine for curing diseases. As therapeutic plants are regular items they are liberated from reactions, they are nearly sheltered, eco-accommodating and locally accessible. Generally there are heaps of herbs utilized for the aliments identified with various seasons. There is a need to elevate them to spare the human lives. However, the blind dependence on synthetic is over and people are returning to the naturals with hope of safety and security. It's time to promote them globally. The result of present study offers a scientific basic for the use of the selected plants *N.arbortristis. P.amarus* and *C.citratus*in the treatment of typhoid fever. These plants species can be regarded as promising resources for anti-typhoid drugs because they showed potent activity against tested bacteria *Salmonella typhimurium*. It can be represented as alternative drug of typhoid.

Authors' Contributions

Gyanranjan Mahalik and Bhagyeswari Behera (Equal contribution as a corresponding author): Conceptualization and designing the research work (Guide & Co-guide); Prangya Paramita Behera, Gyanranjan Mahalik and Bhagyeswari Behera: All authors read, reviewed, and approved the final version of the manuscript.

REFERENCES

1. Hamburger M, Hostettmann K. 7. Bioactivity in plants: the link between phytochemistry and medicine. Phytochemistry. 1991 Jan 1;30(12):3864-74.
2. Hosseinzadeh, S., Jafarikukhdan, A., Hosseini, A., & Armand, R. (2015). The application of medicinal plants in traditional and modern medicine: a review of Thymus vulgaris. *International Journal of Clinical Medicine*, *6*(09), 635.
3. Clark, A. M. (1996). Natural products as a resource for new drugs. *Pharmaceutical research*, *13*(8), 1133-1141.
4. Brusch, J. L., Garvey, T., & Schmitt, S. K. (2010). Typhoid Fever: Treatment & Medication. *World Health Organization (WHO) guidelines Updated*, 1-5.
5. Greenhill, A. R., Guwada, C., Siba, V., Michael, A., Yoannes, M., Wawarie, Y., ... & Horwood, P. F. (2014). Antibiotic resistant Shigella is a major cause of diarrhoea in the Highlands of Papua New Guinea. *The Journal of Infection in Developing Countries*, *8*(11), 1391-1397.
6. Saxena HO, Brahmam M. Flora of Orissa. Vol. 1-4. Orissa: Orissa Forest Development Corporation; 1994-1996.
7. Mahalik, G., Sahoo, S., & Satapathy, K. B. (2017). Evaluation of phytochemical constituents and antimicrobial properties of Mangifera indica L. Leaves against urinary tract infection-causing pathogens. Asian Journal of Pharmaceutical and Clinical Research, 10(9), 169-173.
8. Mbata, T. I., Debiao, L. U., & Saikia, A. (2008). Antibacterial activity of the crude extract of Chinese green tea (Camellia sinensis) on Listeria monocytogenes. *African journal of Biotechnology*, *7*(10).
9. Ravikumar, P. H., Makari, H. K., & Gurumurthy, H. (2001). In vitro antimicrobial activity of ethanol extract of Thevetia peruviana. 6(9), 2318-2322.
10. Rajesh, K., Harsha, R., Ahmed, M. G., Hareesh, A. R., Gowda, S. S. T., Dinesha, R., ... & Ali, M. I. (2010). Antimicrobial activity of ethanol extract of leaf and flower of Spathodea campanulata P. Beauv. *Research Journal of Pharmaceutical Biological and Chemical Sciences*, *1*(3), 691-698.
11. Taylor, J. L. S., Rabe, T., McGaw, L. J., Jäger, A. K., & Van Staden, J. (2001). Towards the scientific validation of traditional medicinal plants. *Plant growth regulation*, *34*(1), 23-37.
12. Farnsworth, N. R., & Bunapraphatsara, N. (1992). *Thai medicinal plants recommended for primary health care system*. Medicinal Plant Information Center.
13. Kunle, O. F., & Egharevba, H. O. (2009). Preliminary studies on Vernonia ambigua: phytochemical and antimicrobial screening of the whole plant. *Ethnobotanical Leaflets*, *2009*(10), 2.

Table 1. Antibacterial activity of ethanol extract of *N. arbour-tristis*, *C. citratus* and *P. amarus* using agar well diffusion assay (ZOI)

Plants	Solvents	Concentration (mg/ml)	Diameter of zone of inhibition (mm) of *S. typhimurium*
N. arbour-tristis	Ethanol	1.0	25
		0.5	-
P. amarus	Ethanol	1.0	15
		0.5	13
C. citratus	Ethanol	1.0	19
		0.5	-

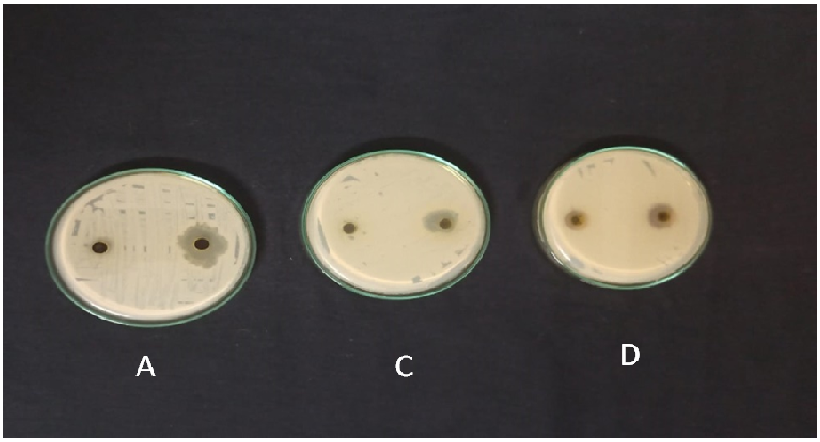

Fig.1. Antibacterial activity of ethanol extract of A. *Nyctanthus arbour-tristis* B. *Cymbopogon citratus* C. *Phyllanthus amarus* leaves using agar well diffusion method in two different concentration (a) 1.0 mg/ml (b) 0.5 mg/ml against *Salmonella typhimurium*

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REVIEW ARTICLE

A Review on Determination of Heavy Metals in the Sum Hospital Area of Bhubaneswar, Odisha: A Step towards Reducing Pollution

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ABSTRACT

Pollution is defined as contamination of the environment due to human activities such as addition unwanted substances of air, land, water etc. Now a day there has been a significant degradation in environment quality. Sum hospital is one of the important hospitals in Odisha and there has been a rapid increase in pollution level within 3-4 years. The increase in the pollution in the environment has resulted in increase in the amount of heavy metals in the our surroundings that has in turn gets absorbed and accumulated in the plants and leads to various deleterious effect on all living organisms.

Keywords: Environment, Plants, Pollution, Contamination, Heavy metals

INTRODUCTION

Biodiversity sustains human livelihoods and life itself. An anticipated 40 per cent of the global economy is based on biological products and processes. As the biodiversity harbors a great amount of diversity with esteem to species diversity, crop diversity, etc. which provides a rich amount of a well evolved system over time background support for rich resources. Nature is a key for the existence of human life. It is a store house of thousands of products essential for our survival. It provides the three most basic necessity i.e food, shelter & clothes. Hence it is necessary for the conservation of nature**.** But the increased human activities haslead to the increase in the environmental exploitation. Increase in the amount of pollution, increased urbanization, industralisation, commercialization etc, change in lifestyle, has contributed in the increase in the level of heavy metals in the environment that has given rise to serious problems like cancers & other chronic diseases in the humans and other living forms. It also has resulted in different changes in the plants (1).

Heavy metals refers to a group of metals that has the atomic mass density of 4g/cm^{3}or greater and isfive times or more greater than of the important liquid for survival i.e water. The increasing amount of toxicity of the heavy metals is becoming a serious problem for ecology, nutrition and as well as for the environment. It has now become evident that, manufacturing, construction activities etc which involves the disposal of materials containing these metals into the environmenthave triggeredan epidemic environmental metal poisoning. These poisonous and toxic substances (metals) cannot be easily degraded using biological systems. These substanceshas a very long half-life period in the environment and biological organisms; thus, they posse an environmental threat. Plants can take up avariety and enormous amount of elements from soil, of which some do not contain any knownbiologically important functions and many are known to be toxic evenat very lower concentration. As the plants are known as building pillar of the ecological food chain; some concerns has been raised about the possibility of presence of certain toxic concentrations of heavy metals being transported from the plants to higher level of the ecological food chain system. The plantscan uptake the toxic metal elements such as Arsenic (Ar), Cadmium (Cd), Chromium (Cr), Mercury (Hg), and Lead (Pb) and could possibly transfer them into the food chain have affected a wide array of living organisms. These elements are very well-established as being extremely toxic in the living body and their effects in human beings are well-known. The leaves are the most susceptible part of a plant to injury because of the presence of large number of stomata which helps in permittance and penetration of pollutants along with heavy metals into the cells and tissues of the leaves (2).

According to Nabulo et al. (2009), the presence of boundary layer resistances acts as the first line barrier against gaseous air pollutants which varies with a number of factor including wind speed, size, shape and orientation of leaves. This pollutant enters the leaves in large number at high wind velocity because the boundary layer resistance gets declined. The presence of waxy cuticle acts as the most potential barrier to most of these pollutants but the cells which are mostly exposed to air pollutants action are the cells of the epidermis. However, the cuticular waxes can get dissociated by acidic gases. These acidic gases could enter the leaves through penetrating the cuticular regions of the leaves. Similarly the heavy metal accumulating and migrating in the soil can enter the plants by the absorption mechanism of the roots and vascular system (3). The plants that grow on the roadside are exposed to high amount of heavy metal pollution due to heavy vehicular emission. It is rightly said by Wang et al., 2015 (4); that the heavy metal produced from vehicular emissions may get accumulated in plants growing in roadside from the soil. Similarly many researchers like Nabulo et al. 2009, Shahid et al. 2017 (3, 5) have told that the airborne heavy metals can be deposited and absorbed via leaves.

According to Chen et al. 2010; Ugolini et al. 2013 (6, 7) heavy metals such as Cadmium (Cd), copper (Cu), and lead (Pb) could have been originated from engine oil consumption, tires, brake wear, and road surface substances. The heavy metals coming out from traffic emissions has tendency to be accumulated in the soil before it gets absorbed by the roots of the plant.As the heavy metals are persistant as well as very resistant thus they can stay in the plant for a longer period of time (8).These thus can get transferred into living human beings (Homo sapiens) through the food chain occurring naturally in the ecosystem (6). The bioavailability of these heavy metals gets mostly affected by the physical-chemical properties of the soil (9) and it is also dependent upon the species of plant under consideration (10-12). In 2016, Chandrashekara and Thasini said that few roadsideplantsare edible while some others have medicinal uses (15). Plants such as *Athyrium esculentum*, *Diplazium esculentum* etc. are edible and plants like *Chromolaena odorata* (Tivragandha) is known for theirmedicinal values (13, 14). Recently researchers Nabulo et al. 2006; Galal and Shehata 2015, are mostly concerned and focused upon the significance of types of soil, theuptake of heavy metals and their accumulation in natural as well in humanmade conditions. The interaction between different heavy elements has led to different harmful effects on the natural environment and its living components (3, 15).

STUDY AT URBAN GUANGZHOU, CHINA

The levels of copper (Cu), nickel (Ni), zinc (Zn), lead (Pb) and chromium (Cr) were measured from the soils and plants growing in urban regions of Guangzhou, China. Here the plant and the soil samples that were collected from the roadside, parks and a university campus and were examined. The average concentrations of Cu, Ni, Zn, Pb and

Cr in the leaves of the plants were about 28.3, 7.7, 142.1, 23.4, and 195.1 mg/kg respectively. In a comparison of heavy metal concentrations in the leaves of the treesgrowing in roadside and park areas, lead (Pb) concentrations was very much higher for roadside plants. However the concentrations of heavy metals was significantly lower for the roots as compared to that of the leaves. This indicated that heavy metal pollution of trees is mostly occurs due to air pollution. Similarly for all top soil samples collected from different regions the average concentrations of Cu, Zn, Pb, Ni and Cr were 24.3, 121.5, 63.9,17.3 and 88.7 mg/kg, respectively (16). Thus it is very evidient that the heavy metal concentrations of the roadside soilsand as well as their coefficient of variation was higher than those in urban parks. By comparing heavy metal concentrations in trees and soil between urban Guangzhou andof Hainan Island, China, Cu, Ni, Zn, Pb and Cr levels in soils and plants in urban Guangzhou were mostly affected by the human impact (17).

STUDY AT JENGKA, PAHANG, MALAYSIA

The uptake and translocation of Cd, Cu, Fe and Pb in different parts of three roadside plants namely *Athyrium esculentum*, *chromolaena odrata* and *lantana camara* growing in semi urban of Jengka, Pahang, Malaysia was observed. Iron (Fe) showed the highest heavy metal concentration of < 850 mg/kg while cadmium (Cd) showed lowest concentration of <0.12 mg/kg. Similarly the heavy metal concentration in the roadside plants was higher than those of plants in the uncontaminated or less unpolluted regions. The PCA (Principal compound analysis) suggests that the sources of natural and manmade sources of heavy metals. The plant roots showed high concentration of Cd and Pb, while the leaves mostly absorbed and accumulated Cu and Fe. The translocation of these four metals suggested that absorption ofthese metals in the above plants have the rank of root >stem >leaves. The metals in the root zone transported weakly to the stem while they get strongly mobilised to the leaves when available in the stem (18).

STUDY AT TOKAT, TURKEY

The heavy metals concentration in the soil, plant and mushroom samples collected from the regions of Tokat, Turkey can be determined by flame and graphite furnace atomic absorption spectrometry after they have bee dry ashed, wet ashed and followed by microwave digestion. The sample preparation procedures showed that the microwave digestion was the best method.This was followed by calculation of Metal accumulation for both the mushroom as well as the plant samples. Higher the ratio of plants to soil cadmium, zinc and copper concentrations indicated that these elements are accumulated mostly by mushrooms samples (19).

STUDY IN INDIA

The issue of metal contamination is becoming a major problem in India. There are many cases of heavy metal toxicity documented in fields of agriculture, mining, power plants, etc. Major environmental heavy metal pollutants mostly in the areas of high human activity areas are cadmium, copper, lead, chromium, mercury etc. The accumulation of heavy metals in the soil is a major source of concern in the productivity of the agriculture as it has adverse effects on food safety and marketability, crop growth due to the effects of phytotoxicity and the health of the living organisms residing in the soil. Toxicity caused by heavy metals has a high impact on plants and consequently has effects on the ecosystem as plants acts as an integral part. The plants growing in highly metal polluted areas shows altered metabolic activities, reduction in the plant growth, low production of biomass as well as accumulation in the heavy metals. Investigation related to toxicity and tolerance of metal stressed plants has prompted by cumulative growth of heavy metal pollution in the environment. Some metals are highly important for the plant growth and metabolism and are present in them in small traces like Cu, Mg, Co, Zn, Cr etc. So, toxicity only occurs if and only the above metals are present in bioavailable forms and at extreme levels (20).

The better effects of nitrate as well as the ammonium ions on different levels of chromium toxicity in 5 year old Sonalika wheat seedlings were studied. Here the growth was measured using both fresh as well as dry weight ; also evaluation of concentration of different contents of chlorophyll, carotenoid, nitrate reductases, peroxidases, catalases etc. there is a decrease in the length of root length in seedling grown without nitrogen was observed. But increase in chromium by 0.001mM has increased the root growth (21). Similarly studies carried out to study the effect of zinc on the growth, accumulation of proline, production of the free radical in the shoots of *Brassica juncea* and *Cajanus cajan*.

Here the seedlings of the above plants was grown in modified B5 medium that was supplemented with zinc sulphate under controlled sterile conditions. A very small amount of zinc (up to 0.1 mM) is seen to enhance the growth of seedlings in both the plants. However, in contrast to production of free radicals that is measured in terms of malondialdehyde as well as the relative level of proline were low in the seedlings raised in the presence of these concentrations of zinc. But presence of zinc at relatively higher concentrations is proved to decrease the growth, but has resulted in increase in the generation of free radicals as well as the accumulation of proline in these plants (22).

CONCLUSION

Plant development and advancement can be unfavourably influenced by unnecessary measures of substantial metals take-up as apparent by research up until now. Contamination of natural habitat because of different anthropogenic exercises is a test for creating nations like India. This has straightforwardly or by implication prompted the expansion in the measure of substantial metals in the environment. The significant sources are vehicular outflow, modern emanation, development exercises, and so on. Because of these exercises the measure of destructive harmful metals like Hg, Pb, As, and so on are expanding in nature which contributes towards are the significant source of heavy metal pollution. Presently a day numerous logical explores are occurring so as to discover a reasonable answer for this issue. Researchers are currently a day's amassing in discovering choices and options so as to bring down the measure of heavy metal outflow into the environment. As a piece of such finding utilization of green and safe energize water and common gases as fuel in various anthropogenic activities that are required for improvement of our country have added to bring down the outflow of such substances in nature.

REFERENCES

1. Mahalik G, Satapathy KB. Environmental impacts of mining on biodiversity of Angul - Talcher open mining site, Odisha, India Scholars Academic Journal of Biosciences.2016; 4(3A), 224-227.
2. Rai PK. Biodiversity of roadside plants and their response to air pollution in an Indo-Burma hotspot region: implications for urban ecosystem restoration. J Asia Pac Biodiversity. 2016; 9:47-55.
3. Nabulo G, Oryem-Origa H, Diamond M .Assessment of lead, cadmium, and zinc contamination of roadside soils, surface films, and vegetables in Kampala City, Uganda. Environ Res. 2006; 101:42–52.
4. Wang D, Dang Z, Feng H, Wang R. Distribution of anthropogenic cadmium and arsenic in arable land soils of Hainan, China. Toxicological & Environmental Chemistry. 2015; 97(3-4):402-8.
5. Shahid M, Dumat C, Khalid S, Schreck E, Xiong T, Niazi NK. Foliar heavy metal uptake, toxicity and detoxification in plants: a comparison of foliar and root metal uptake. J Hazard Mater. 2017; 325:36–58.
6. Chen X, Xia X, Zhao Y, Zhang P Heavy metal concentrations in roadside soils and correlation with urban traffic in Beijing, China. J Hazard Mater. 2010; 181:640–646.
7. Ugolini F, Tognetti R, Raschi A, Bacci L. *Quercus ilex* L. as bioaccumulator for heavy metals in urban areas: effectiveness of leaf washing with distilled water and considerations on trees distance from traffic. Urban For Urban Green. 2013; 12(4):576-584.
8. Boularbah A, Schwartz C, Bitton G, Aboudrar W, Ouhammou A, Morel JL Heavy metal contamination from mining sites in South Morocco: 2.Assessment of metal accumulation and toxicity in plants. Chemosphere. 2006; 63(5):811-817.
9. Liu WX, Shen LF, Liu JW, Wang YW, Li SR. Uptake of toxic heavy metals byrice (*Oryza sativa* L.) cultivated in agricultural soil near Zhengzhou city, People Republic of China. Bull Environ Contam Toxicol. 2007; 79:209-213.
10. Koz B, Cevik U. Lead adsorption capacity of some moss species used for heavy metal analysis. Ecol Indic.2014; 36:491-494.
11. Keshavarzi B, Moore F, Ansari M, Mehr MR, Kaabi H, Kermani M. Macronutrients and trace metals in soil and food crops of Isfahan Province, Iran. Environ Monit Assess. 2015;187(1):4113.

12. Zhao S, Duo L. Bioaccumulation of cadmium, copper, zinc, and nickel by weed species from municipal solid waste compost. Pol J Environ Stud. 2015; 24(1):413-417.
13. Chandrashekara UM, Thasini VM. Non-crop edible plants and medicinal plants in Home garden Agroforestry System of Palakkad District, Kerala. Int JEcol Environ Sci. 2016; 42(2):183-191.
14. Roslan NA, Syed Ismail SN, Praveena SM. The transfer factor of cadmium in fern leaves and its potential health risk. Asia Pac Environ Occup Health J. 2016; 2(2):48-57.
15. Galal TM, Shehata HS. Bioaccumulation and translocation of heavy metals by *Plantago major* L. grown in contaminated soils under the effect of traffic pollution. Ecol Indic. 2015; 48:244-251.
16. Lu X, Zhang X, Li LY, Chen H. Assessment of metals pollution and health risk in dust from nursery schools in Xi'an, China. Environ Res. 2014; 128:27-34.
17. Liu WX, Liu JW, Wu MZ, Li Y, Zhao Y, Li SR. Accumulation and translocation of toxic heavy metals in winter wheat (*Triticum aestivum* L.) growing in agricultural soil of Zhengzhou, China. Bulletin of environmental contamination and toxicology. 2009; 82(3):343-7.
18. Tanhan, P., Kruatrachue, M., Pokethitiyook, P., & Chaiyarat, R. (2007). Uptake and accumulation of cadmium, lead and zinc by Siam weed [*Chromolaena odorata* (L.) King & Robinson]. Chemosphere, 68(2), 323-329.
19. Dospatliev L, Ivanova M. Determination of heavy metals in mushroom samples by Atomic Absorption Spectrometry. Bulgarian Chemical Communications. 2017; 49:5-9.
20. Tchounwou PB, Yedjou CG, Patlolla AK, Sutton DJ. Heavy metal toxicity and the environment. In Molecular, clinical and environmental toxicology 2012 (pp. 133-164). Springer, Basel.
21. Shanker AK, Cervantes C, Loza-Tavera H, Avudainayagam S. Chromium toxicity in plants. Environment international. 2005; 31(5):739-53.
22. Singh S, Sinha S. Accumulation of metals and its effects in Brassica juncea (L.) Czern.(cv. Rohini) grown on various amendments of tannery waste. Ecotoxicology and Environmental Safety. 2005; 62(1):118-27.

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RESEARCH ARTICLE

Studies on the Effect of Pollution on Avenue Plants in Different Heavy Traffic Area of Bhubaneswar, Odisha, India

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ABSTRACT

Pollution is the introduction of contaminants into the natural environment that causes adverse change. Pollution can take the form of chemical substances or energy, such as noise, heat or light. Pollutants, the components of pollution, can be either foreign substances/energies or naturally occurring contaminants. Air pollution occurs when harmful or excessive quantities of substances are introduced into Earth's atmosphere. Sources of air pollution include gases, particulates, and biological molecules. The effects of air pollution on plants are widely seen and damage all plants including our food crops and trees. In the lower atmosphere, ozone damages plants by preventing photosynthesis and obstructing stomata, restricting respiration and stunting plant growth. In the current studies concentration of heavy metal in different avenue plant sample collected from heavy traffic areas of Bhubaneswar. Four highly traffic area selected were Vani Vihar, Jaydev Vihar, Barmunda (Fir station), Delta square, each sample were collected. The collected leaves were dried and grinded into fine particle the heavy metals were analysed through XRF (X-ray fluorescence) spectroscopy. The result should the accumulation of different heavy metal such as iron, titanium, manganese, copper, zinc, chromium, nickel in the selected area determined.

Keywords: environment, Pollution, photosynthesis, spectroscopy, stomata

INTRODUCTION

Developmental activities give birth the seeds of environmental harm with them, aided and abetted by both needs and greed of man. Activities like as manufacturing, processing, transportation and expenditure of natural resources

not only deplete the stock of natural resources but also add difficulty to the environmental by accumulation of wastes. The term pollution comes from the Latin word 'pollutioneum' which implies to defile or create dirty. According to National Environmental research Council, "Pollution is viewed as the unwariness of substances and energy as waste product of human activities that lead to harmful changes inside the natural environment (1). Growing industrialization and evolution activities is the primary source of pollutant emission into the surrounding and introduce catastrophic substances into the atmosphere (2). Vehicular emissions in developed countries have largely restrained by betterment of vehicle parts and fuel hydrocarbon emissions; nevertheless, it cannot be said for developing countries, where numerous old and poorly serviced vehicles ply the roads joined with the use of low quality fuel. Transportation with the combustion of diesel and gasoline in automobiles has been considered as high source of air pollution, both at regional and international levels. Motor vehicles release a capacious quantity of exhaust emission such as carbon monoxide (CO), sulphur dioxide (SO_2), nitrogen oxide (NO_x), volatile organic compounds (VOCs) and particulate matter that commute 60-70% of the air pollution found in a city area (3).

Numerous industrial plants and burdensome traffic may create heavy metals and different poisonous compounds into the air that may create harmful health effects in man or animals; affect plant life and effect the worldwide surroundings by changing the air quality of the earth (2). There is no mechanical or chemical instrument, which can completely analyze the emission of pollutants at the source. Once the pollutants are free to the air, exclusively the plants are the only hope, which can mop up the pollutants by adsorbing and metabolizing them from the air. Hence the plants, role abatement are progressively acknowledged in recent period. Plants act as a sink or as living filters to decrease air pollutant by processing characteristic response and symptoms (4, 5). Moreover, roadside plant leaves are in direct contact with air pollutant, and can accumulate some amount heavy metals. The current study aims to find out the accumulation of heavy metals in road side plants of heavy traffic area of Bhubaneswar city of Odisha.

MATERIALS AND METHODS

Study area

Bhubaneswar is a very old city in India's eastern state of Odisha, formerly Orissa. The city is lying between 20° 15' N latitude and 85° 52' E longitude. Four heavy traffic areas were selected for the studies which were coded As Site-A, Site-B, Site-C and Site-D. Site-A: Barmunda, Fire Station area, located in latitude 20.2790° N, and longitude 85.7993° E. Site-B: Delta Square, located in latitude 20.2755° N, and longitude 85.8039° E. Site-C: Vani Vihar, located in latitude 20.2930° N, and longitude 85.8533° E. Site-D: Jayadev Vihar, located in latitude 20.2997° N, and 85.8173° E.

Plant sampling

Twelve plant samples, three from each site were selected for this study, as they were common along roadside (6). The species are namely *Senna tora, Neolamarckia cadamba, Bauhinia variegata, Ficus religiosa, Delonix regia, Nerium oleander, Mangifera indica, Polyalthia longifolia, Terminalia catappa, Ficus benghalensis*.

XRF Analysis

The plant samples were dried, homogenized and sieved at 250 μm particle sizes. XRF analyzes were carried out at the Advanced Testing and Calibration laboratory in Centurion University Of Technology And Management using a handheld Epsilon 1Pananlytical XRF spectrometer. By automatically adjusting for matrix effects, Epsilon 1 Pan analytical XRF spectrometer analyzers are able to determine the content of soil samples typically in seconds, without any requirement for instrument users to input empirical, sample specific calibrations. The sample name, spectrum and elemental composition are stored in a dedicated library. Each soil sample was analyzed five times for 240 s using two X-ray filters, one for elements from potassium to copper and also the second for elements from zinc to antimony (7).

RESULTS AND DISCUSSION

The present study revealed a decrease in leaf area in all plant species, growing at sites with heavy vehicular traffic site like Barmunda, Delta square, Vani Vihar, Jaydev Vihar (Table 1). The use of automobiles is growing fast globally at large and with much greater pace in developing countries. At global level, there were about 53 million automobiles in the 1950s, which had exceeded to 500 million up to 2000. About 19 million vehicles are added each year to the global total (3). Vegetation offers a large surface area that acts as an important sink for the atmospheric pollutants. Plants can take-up atmospheric gases either without their active metabolism, or actively metabolizing them thus creating a concentration gradient that can facilitate their continuous absorption. While in most cases, the active metabolism of these pollutant gases results into the adverse effects on plants, it may also be beneficial in case of certain pollutants.

From the above table it was found that in sample 1 to 12 have highest concentration of iron oxide (Fe_2O_3) is highest followed by Manganese Oxide (MnO), Titanium Dioxide (TiO_2) Zinc Oxide (ZnO) Copper Oxide (CuO) and Chromium Oxide (Cr_2O_3) .Trace amount of As, Ga, Re, Yb, Eu, Th, Nb, Zr, Y, Rb, V, Ti, Si, etc (Table 2 & Fig.2). Some these heavy metals play vital role in photosynthesis and other metabolic activities and the others are carcinogenic and may cause may cause plant ailments like curling of leaves and early ageing. Elements like Fe, Mn, Zn, Cu, etc. are essential for differ physiological activities of the plant where as elements like As, Cd, Hg are highly poisonous for plants and long term exposure can cause chlorosis (8).

CONCLUSION

The above study concluded that common road side plant species growing at Site A and Site B of Bhubaneswar city suffers maximum because of heavy pollution compared to Site D and Site C. Reduction and increase in various parameters of the plant species studied at selected sites can be considered as an adaption to protect plants against air pollution stress. The present study suggests that the morphological and biochemical traits of selected roadside plant species can serve as suitable bio indicators of particulate pollution and an excellent quantitative and qualitative index of pollution level by capturing significant amount of health- damaging particles from the atmosphere with the potential to perk up local air quality.

REFERENCES

1. Swami A. Impact of Automobile Induced Air Pollution on roadside vegetation: A Review. ESSENCE International Journal for Environmental Rehabilitation and Conservation. 2018; 9(1), 101–116. https://doi.org/10.31786/09756272.18.9.1.113.
2. Rai PK, Panda LLS. Roadside plants as bio indicators of air pollution in an industrial region, Rourkela, India. International Journal of Advancements in Research & Technology. 2015; 4(1), 14–36.
3. Dwivedi A K, Tripathi BD. Pollution tolerance and distribution pattern of plants in surrounding area of coal-fired industries. Journal of Environmental Biology. 2007; 28(2), 257-263.
4. Pandey J, Pandey R, Shubhashish K. Air-borne heavy metal contamination to dietary vegetables: A case study from India. Bulletin of Environmental Contamination and Toxicology. 2009; 83(6), 931–936. https://doi.org/10.1007/s00128-009-9879-1
5. Verma A, Sharma P, Dhusia N, More N. Determination of heavy metal content in fruits and fruits juices consume in urban areas of Lucknow, India. International Journal of Food Science and Nutrition.2016; 1(5), 44–50.
6. Uka UN, Belford EJD, Hogarh JN. Roadside air pollution in a tropical city: physiological and biochemical response from trees. Bulletin of the National Research Centre. 2019; 43(1). https://doi.org/10.1186/s42269-019-0117-7

7. Ene A, Boşneagă A, Georgescu L. Determination of heavy metals in soils using XRF technique. Romanian Reports of Physics. 2010; 55(7-8), 815-820.
8. Nagajyoti PC, Lee KD, Sreekanth TVM. Heavy metals, occurrence and toxicity for plants: A review. Environmental Chemistry Letters. 2010; 8(3), 199-216. https://doi.org/10.1007/s10311-010-0297-8.

Table 1 showing different plant samples collected from Site-A, Site-B Site-C, Site-D

Site-A (Barmunda, Fire Station area): SAMPLE-1, 2, 3	**Site-B (Delta Square): SAMPLE-4, 5, 6**	**Site-C (Vani Vihar): SAMPLE-7, 8, 9**	**Site-D (Jayadev Vihar): 10, 11, 12**
Nerium oleander L.	*Terminalia catappa* L.	*Senna tora* (L.)Roxb.	*Ficus religiosa* L.
Mangifera indica L.	*Polyalthia longifolia* (Sonn.) Thwaites	*Neolamarckia cadamba* (Roxb) Bosser	*Neolamarckia cadamba* (Roxb) Bosser
Polyalthia longifolia (Sonn.) Thwaites	*Ficus benghalensis* L.	*Bauhinia variegate* L.	*Delonix regia* (Hook.) Raf.

Table 2. Pollution index for different study sites during the study periods.

Sl. No	Elements	Sample -1	Sample -2	Sample -3	Sample -4	Sample -5	Sample -6	Sample -7	Sample -8	Sample -9	Sample -10	Sample -11	Sample -12
1.	SiO_2	9.304	3.785	4.773	11.785	14.450	2.667	13.795	31.029	6.044	13.795	31.029	6.044
2.	P_2O_5	4.432	4.038	4.943	2.388	1.684	5.607	2.395	1.823	3.108	2.395	1.823	3.108
3.	SO_3	8.575	5.590	6.539	2.284	2.088	8.748	4.495	2.857	3.846	4.495	2.857	3.846
4.	Cl	3.820	0.656	0.544	0.722	3.350	3.143	6.000	0.451	3.299	6.000	0.451	3.299
5.	K_2O	34.596	33.134	31.730	25.915	23.215	26.638	23.409	11.899	25.641	23.409	11.899	25.641
6.	CaO	32.076	48.014	46.719	54.739	48.349	49.915	40.089	47.241	51.859	40.089	47.241	51.859
7.	TiO_2	0.825	0.427	0.151	0.246	0.681	0.304	0.912	0.383	0.574	0.912	0.383	0.574
8.	V_2O_5	0.026	-	0.0136	-	0.01635	0.00583	0.02339	0.00678	0	0.02339	0.00678	0
9.	Cr_2O_3	0.07239	-	0.05748	0.00846	0.05763	0.03357	0.103	0.03644	0.159	0.103	0.03644	0.159
10.	MnO	0.279	0.387	0.126	0.124	0.822	0.326	0.918	0.415	0.269	0.918	0.415	0.269
11.	Fe_2O_3	5.700	3.549	3.737	1.388	5.027	2.248	7.412	3.608	4.898	7.412	3.608	4.898
12.	NiO	0.0149	-	0.00939	-	-	-	-	-	0.01042	-	-	0.01042
13.	CuO	0.04235	0.06543	0.08095	0.07695	0.04417	0.0426	0.0803	0.04872	0.06804	0.0803	0.04872	0.06804
14.	ZnO	0.0321	0.05835	0.05972	0.03944	0.112	0.09784	0.145	0.07192	0.06107	0.145	0.07192	0.06107
15.	As_2O_3	-	-	-	-	0.00098	-	-	0.0012	-	-	0.0012	-
16.	Br	0.00555	-	-	0.00196	0.00753	-	0.01038	0.00228	0.00695	0.01038	0.00228	0.00695
17.	Rb_2O	0.01639	0.02624	0.01571	0.02347	0.02464	0.01834	0.05821	0.01295	0.02638	0.05821	0.01295	0.02638
18.	SrO	-	0.02888	0.0146	0.06577	0.04299	0.01129	-	0.0521	0.0352	-	0.0521	0.0352
19.	ZrO_2	-	-	-	0.0017	0.01111	-	0.02111	0.01047	0.00827	0.02111	0.01047	0.00827
20.	CeO_2	-	0.06928	-	0.08669	-	-	-	-	0.0319	-	-	0.0319
21.	SnO_2	0.180	0.168	0.124	0.02404	0.01439	0.193	-	-	-	-	-	-
22.	Eu_2O_3	-	-	-	0.07754	-	-	0.130	0.0489	0.0505	0.130	0.0489	0.0505
23.	Er_2O_3	-	-	-	0.00245	0.00008	-	-	-	-	-	-	-
24.	Os_4	0.00138	-	0.00008	-	-	-	0.00401	-	-	0.00401	-	-
25.	Yb_2O_3	-	-	-	0.00046	-	0.00068	-	-	0.00265	-	-	0.00265
26.	PtO_2	-	-	-	-	0.00305	-	-	-	-	-	-	-
27.	PbO	0	0	0	0	0	0	-	0.00274	-	-	0.00274	-
28.	CO2	0.00023	0.0042	0.00061	0	-	0.0007	0	0	0	0	0	0
29.	Re							0.00084	0	0.00132	0.00084	0	0.00132

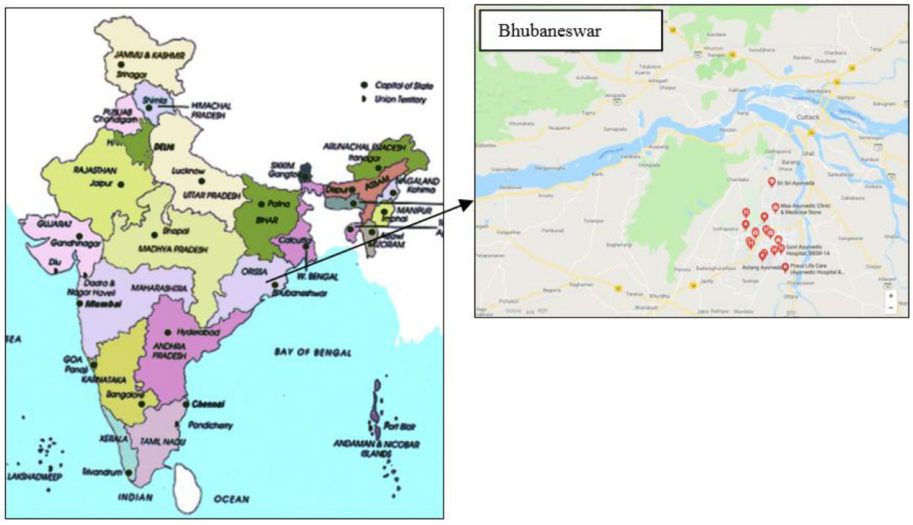

Fig 1: Map showing study area

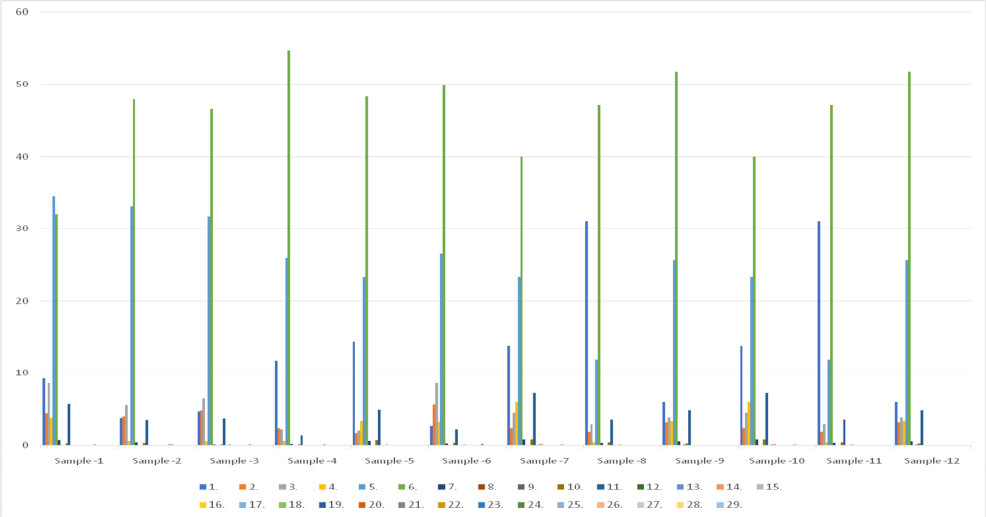

Fig.2. Concentration of different elements present in study area [Sites-A, B, C, D in percentage (%)]

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REVIEW ARTICLE

Ethnobotanical Survey and Antimicrobial Activity of Medicinal Plants Used To Cure Various Diseases in Kaptipada and Udala Block of Odisha, India: A Review

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ABSTRACT

This paper presents a review of various plants identified from different botanical surveys and folklore medicinal surveys with antimicrobial properties. In the developing country conventional medicinal plants are the main part of the initial health care setup. The ethnobotanical survey updating knowledge about herbal medicine to cure different infectious diseases. It mainly points of convergence on the relation between local inhabitants and indigenous plant. This review discusses medicinal plants, their habit, preparation of drugs, and mode of application with their botanical identification. The plant parts used in the form of paste, powder, decoction, juice, infusion and also in crude form, with other additional like curd, urine, cow milk, and honey to cure various disorders including backache, burn, fever, cough, diarrhea, headache, malaria, post-partum, sprain, stomachache, wound, joint pain, diabetes, vascular disorders, antibacterial, antifungal, etc.

Keywords: Antimicrobial, Decoction, Ethnobotanical, folk, Medicinal, Infections

INTRODUCTION

Ethnobotany is defined as traditional use of medicinal plant and the study of the relationship between of plant and local people. It mainly points of convergence on the relation of local plant and local people. Herbal use in our country has long historical convention. This conventional awareness reported by teacher, physicians, student of university, naturalists, and professor during 19th and 20th centuries. This ethnobotanical studie give information

awareness about herbal medicine in Udala and kaptipada area of Mayurbhanj district. The most ethnobotanical studies report on the important plant families use as medicine and drugs (1).

In the developing world traditional medicinal plant are important part of the primary health care system. The ethnobotanical survey to give different information for prepare of drugs to treat human and animal illness. Now a days various disease are treated for using the herbal remedy without any side effects. In many countries human beings are trust on conventional awareness and medication plants for their initial health care. Many people are depending on local plant resources for medicine. But this conventional awareness is decrease, so it is preserved in various forms for future generation. This survey aimed to give detailed information of these plant and their medicinal properties (2). Ethnomedicinal studies are of the important cost to find simultaneous drugs from local medicinal plant resource. The information of conventional awareness of indigenous plant species has supply a number of medicines. The natural remedy value is very high to discover new contemporary drugs (3).

Antimicrobial activity defined as the process of kill the infection cause microbes. Antimicrobial may be anti-fungal, anti-viral, anti-bacterial. All are different, they act to restrain the disease. As long as historicism, people has found antimicrobial activity of plant to treat contagious diseases and some of these herbal remedy as part of the require of different disease (4). Due to antibacterial and antioxidant activities of various medicinal plants has increase during last decagon. Ascertainment the antimicrobial activities of various medicinal plants is interest due to current global issue of high antibiotic power of microorganism. It is accepted that the drug hostility in microorganism is grow to use of trade antimicrobial drugs (5).

Through pharmacological industries have make number of new antibiotics for recovery of different disease. Plant are the important sources of nature and it help both animal and human beings to cure various diseases. The plants extract and phytochemicals both with have antimicrobial properties, and it can use to treatment (6).

Ethnobotany

Ethnobotanical survey defined as the details on therapeutics use of medicinal plant by tribal area. The "therapeutics medicine" give better knowledge or information based on theory and trust local inhabitants that are use to improvement of health, to prevention of diagnosis and treated various diseases. In the world approximate all plant play a main role to prevention of different diseases. Ethnomedicinal or ethnobotany studies are providing information to identify new medicinal plant and their beneficial activity (7).

Mostly indigenous people are used plants for food, fuel, to prepare drug for prevention of disease, agrochemicals, pharmaceuticals and various purposes. The plant part have been use in the form of juice, power, paste, decoct, curd form and infusion, with other addition like honey, urine cow milk and curd to relaxation of various disease like skin disease, urine infection, diabetes, inflammations, wounds, skin problem, pimples, fever, snake bites, cough, dental problems, hair fall, skin wrinkle, worm and other disease (2).

The ethnobotanical survey was first focus on herbal remedy oral history make use by nomad people of a region, recognize new herbal plants and utilize them for prepare drug. This study to distributed different knowledge and various information about medicinal plant or herbal remedy in the indigenous community (8).

Antimicrobial activity means to kill the microorganism and stop their growing. In advanced realm importantly in India poor people such as farmers, people of villages and local inhabitants use progenitor medicine for treatment of infection. The plant parts have been uses in the form of decoction, juice and teas to treated different infectious disease. More people trust healers and shamans cause of their experience to prepare herbal remedy for treatment of different infectious disease because the herbal remedy have antimicrobial activity (9).

Abroad

Bulgaria

In Bulgaria herbal remedies uses has a long conventional. This conventional awareness described during 19th and 20th country by university professors, lecture, teacher, naturalist, physicians and folklorists. The conventional awareness growing fast. The ethnobotanical survey to give detail information about medicine in Bulgaria (10).

China

The medicinal plants are uses to recover various disease in all over in world. In China people are use traditional drug to prevention of disease. For example, Tibetan medicine are popular to cure digestive problem,rheumatic problem and wounds etc. The Mongolians medicines are more effectual to prevention of brain shock and bone fracture. Yao medicine are use to cure cancers and skin problems. The Maonna people depends medicinal plant for self-medication. Local inhabitants are using endemic species and they have developing their own conventional awareness. Oral history the Maonan people described their conventional awareness from generation to generation without written form (11).

Bolivia

The ethnobotanical survey of medicinal plants in Bolivia documented 31 tribal community and many mestizo communities living in different area of the country, as Altiplano, Yungas, Chaco or Lowlands. This paper reported about 129 species, belonging to 55 vascular plant families and 1 lichen family. The most major plants are Asteraceae 22 species, Fabaceae 11 species and Solanaceae 8 species. More than 90 medicinal plants are use to cure different disease such as digestive system disorders (stomach ailments and liver problems), musculoskeletal body system (rheumatism and the complex of connotations, luxations, sprains, and swellings), gynecological disorders (12).

Greece

In thousand years old the medicinal plants are use to remedy for cure illness in Greece. The folk medicine are uses in Greek. An historical study the awareness of medicinal plants of Greece documented some information about most valuable plants use in folk medicine in Greece (13).

India

In India different people are live together of tropical regions, vegetation and climate. In ethnobotanical survey of India has old history. In India basically two communities those live small cities or rural area or village and tribal people of India provide more information about botanical survey in India (14). Ethnobotany is the part of ethnobiology and the ethnobotanical survey are the main part for restore the conventional awareness about 85% of herbal medicine use for preliminary health care system. The India has more ethical awareness commonly 500 indigenous cliques belong to 227 ethic group. In India the indigenous people are rely in herbal remedies for cure diseases. The ethnobotanical survey to collect data about medicine used in South India for respiratory disease. The present data documented the indigenous people of south India state like Andhra Pradesh, Karnataka, Maharashtra, Kerala and Tamil Nadu. 90 plant species to cure respiratory disorders. The most common reported species are *Adhathoda vasicanees*, *Tylophora indica*, *Datura metal*, *Clerodendrum serratum*, *Terminalla chebula*, *Leucas aspera*, *Ocimum sanctum* (15).

Tamilnadu

India has more then 427 indigenous groups and the present paper are gives information about traditional medicinal knowledge in Vellore district Tamilnadu. The world health organization (WHO) about 60 to 80% of people are trust in herbal drug and this data are found in old literature like Charak Samhita, Sushruta and Samhita, Atharveda etc. About 2500 medicinal plants 100 species are use common drugs and cure different illness like cardio vascular

disorders, hepatoprotective, antifungal disease, antibacterial disease, wound and diabetes etc. In globe 20,000 plants are use as drug; these data are given by WHO (16).

Tripura

Tripura is a state of India and a part of both Himalayan and Indo-Burma biodiversity region. In this state more medicinal plants are use to cure various disease, 19 tribal in Tripura are rely on Natural plant medicine. In this survey provided that 113 medicinal plant species from 56 families with their local name, botanical name, family, habit, application and medicinal properties etc. Out of 56 families, the important families are Euphorbiaceae (7 species), Apocynaceae (6 species), Fabaceae and Rubuaceae (each 5 species), Liliaceae, Asteraceae, Verbenaceae and Caesalpiniaceaer (each 4 species), Labiate, Zingiberaceae , Combretacare ,Malvaccae and Rutaceae (3 speciaes each) (17).

Andhra Pradesh

The ethnobotanical survey of medicinal plants used by Kaya tribes of medaram and narlapura villages, of South of the Godavari river, Thadvaimandal, Warangal district, Andhra Pradesh, India. 34 plant species belonging to 24 families, this data was collected by local people between age of 35-78. They have been using these plants to cure different diseases like inflammations, dental problem, skin infection, headache, indigestion, urinary infection, fever, snake bite and cough (2).

Odisha

Odisha is another state of India & the state has richest medicinal plant & Natural resources. More tribal community is live together. It has the 3rd highest tribal populations numbering over 8 million. The local inhabitants to know about indigenous plant to cure diseases (18).

Koraput

Koraput is the district of Odisha. This ethnobotanical survey was documented 50 species of plant that use in our daily needs and the most important family are Euphorbiaceae and Myrtaceae. Other documented plants are *Curcuma montana*, *Cardiospermum helicacabum*, *Caryota urens*, *Sansiveria roxiburghina*, *Atylosia scarabaeoide*, *Argyreia speciose*, *Sesbania grandiflora*, *Stephania hernandifolia*, *Elephantopus scaber* etc (19).

Khordha

Khordha is the district of Odisha. This ethnomedicine are documented folk medicinal uses of plant to cure different disease. Khordha district is situated in the southwest of the state and it touch the Chilika lake in the south. The district has village/town like Mangrajpur, Shaktihal, Pratap, BanpurJodamdosahi, Khariabandho, Dhuanali, Bhaliapoda, Kudubibadi, Bhaliapada, Kudubibadi, Bhenuambadi, Kumanipani, Dykechhak, Saliadam etc. Kumar et al., recorded some 54 folk recipes, 43 taxa of folk medicinal plant used by Kondh, Sabra, Tribes, Naik of the area for cure different diseases (18).

Kandhamal

Panigrahy et al., worked in Kandhamal district and found mostly two tribal community i.e. dongria and desia are dominate. They speak Kui language. The ethnomedicinal information was documented in kui language. They know various plant and their particular uses for cure diseases. They recorded the 40 ethnomedicinal plant species, 37 genera and 28 families with their botanical identification. These ethnomedicinal plants used in gastrointestinal disease, cold, dysuria, skin disease and cough etc (20).

Sundargarh

Sundargarh district are near in Ranchi district of Jharkhand state, Raigar district of Chattisgarh, Jharsuguda, Sambalpur in Odisha. This ethnobotanical paper gives better information for new drugs, food, natural product, chemicals, pesticides & other. In this area have vast forest, rocky area, river and hill. The important river is Ib and

Brahmani and the district have goldmine of natural medicine plants. Mostly 40 ethnic tribal communities are leaves in this area and they have full knowledge about herbal medicine. The most important tribals are Kharia, Kisan, Bhoiyan, Oraon, Munda and Gond. Documented 83 plant species with 78 genera in 42 families (21).

Malkangiri

Biswas et al., documented 35 plant species with their proper identification like local name, botanical name, habit, mode of methods, and application etc in Malkangiri (22).

Nawarangpur

The district is situated in Odisha state and the districts have rich diversity of ethnobotanical species and it given benefits from social and economic needs. The people of these districts are use plants to treated different disorders. Most of plant are destroyed or extinction in this area. According to the World Health Organization (WHO), 65% of the world's populations well know the value of plants for initial health care system. Today 25% of medicine are prescribed are come from various plants. During study a total number of 69 plant species belonging to 43 families are reported (23).

Coastal Districts

Sahu et al. work on costal district like Balasore, Bhadrak, Jagatsinghpur, Jajpur, Kendrapara etc. In the coastal area most major river is the Budhabalanga, the Suvarnarekha, the Rushikulya, the Baitarani and the Mahanadi. The costal line is the gift of 6 river. During the work they documented 46 plant species belong to 44 genera and 32 families with their botanical identification and the plant majorly cure jaundice, diarrhea, piles, urinary trounles and skin disease (24)

Mayurbhanj

In the state of Odisha Mayurbhanj is the largest district and it explant over 10,418 sq. km and the forest area cover 4392.13 sq. km in the district. The district is bounded Singhhum, Saraikela, Jharkhand, Madnapur and Keonjhor, Balasore etc. The Similipal Biosphere Reserve (SBR) are situated in the center of the district. The old men women and Vaidya Kaviraj have good knowledge about herbal medicine. They documented 380 plant species, 23 plants belongs to 22 genera and 18 families are used to cure of joint diseases (arthritis, rheumatism, lumbago and gout). Rheumatism, arthritis, lambago and gout disease are common in this area and if don't treated instantly then the joint problem become chronic (25).

The large numbers of plants were used by the tribes and local healer to cure various diseases. The details are given in table 1.

Antimicrobial Activity

Many plants and their parts are use as medicine for their antimicrobial properties to cure various infectious diseases. These studies aimed on survey of antimicrobial activities of plants and are use as different medicine. The result showed that 4 different plant extracts was concealed in opposed to 12 pathogenic microorganism and some plant like Methanolic extracts of *Oxalis corniculate, Artemisia vulgaris, Cinnamomum tamala* etc. expose to antimicrobial activity by agar. *Ageratina Adenophora* show antifungal activities in opposed to Rhizopus spp. Antimicrobial activity of plant reduce infectious disease in world. More medicinal plants are identified for the treatment of bacterial infection. According to the (WHO) plants are the important source to preparation of drugs (31). The Chatkal Biosphere Reserve of Uzbekistan the endophytic bacteria isolated from two medicinal plant i.e. *Hypericum perforatum* and *Ziziphora capitate* with antimicrobial activities. The plant extract of *H. perforatum* have in opposed to bacterial and fungal pathogens but *Z. capitate* did not have antimicrobial property (32). Dabue et al., reported antimicrobial activity of 24 plant of 77 extracts was concealed in opposed to 8 bacteria and 4 fungi using microbroth dilution. The water extracts of plants are better in opposed to the bacterial and fungal infection & this study aimed the antimicrobial activity of medicinal plant used in Ayurvedic medicine for fungal & microbial infection (33). During 1966 to 1994 the survey

found 115, in between 1995 to 2004 the survey documented 307 antimicrobial activity of plant species to use in folk medicine. The indigenous use plants to cure micro-bacterial, fungal infection like the use of bearberry and cranberry juice to cure urinary infection and lemon balm, garlic and tee tree are use to treat infectious other to treat, respiratory system, gastrointestinal and biliary system on skin infection etc (34).

Salhi et al., In Northern Sahara of Algenia the study documented the antifungal activity of extracts from local plants. The fungal activities of these plants to control 2 fungal species belong to *Fusarium* in vitro assay. The fungal infections in cereals have more criteria like lowering of yield capacity, low their nutritive value etc. The most valuable fungi attack the yield of small grain in cereal and causing spoilage. Various remedy to use to control of fungal disease. Recently approximation 200 species of plant are chemical pesticides have different side effects (35).

CONCLUSION

This review of literature reveals that therapeutic plants utilized for the treatment of different diseases in Kaptipada and Udala block of Odisha are expected to report the indigenous practice and fill in as logical benchmark data for future studies. Sharing of such information is critical for keeping up choices for the utilization of traditional medicines, especially as utilization of elective medication is developing a result of low expenses and biomedical significance. The greater part of the therapeutic plants was reaped from the wild that the characteristic living spaces should be overseen appropriately to limit the dangers of restorative plants sooner rather than later.

REFERENCES

1. Koleva, V., Dragoeva, A., Nanova, Z., Koynova, T., & Dashev, G. (2015). An ethnobotanical study on current status of some medicinal plants used in Bulgaria. *Int. J. Curr. Microbiol. App. Sci*, *4*(4), 297-305.
2. Manjula, S., & Mamidala, E. (2013). An ethnobotanical survey of medicinal plants used by traditional healers of Thadvai, Warangal district, Andhra Pradesh, India. *International Journal of Medical Research & Health Sciences*, *1*(2), 40-46.
3. Umair, M., Altaf, M., & Abbasi, A. M. (2017). An ethnobotanical survey of indigenous medicinal plants in Hafizabad district, Punjab-Pakistan. *PloS one*, *12*(6), e0177912.
4. Rios, J. L., & Recio, M. C. (2005). Medicinal plants and antimicrobial activity. *Journal of ethnopharmacology*, *100*(1-2), 80-84.
5. Farjana, A., Zerin, N., & Kabir, M. S. (2014). Antimicrobial activity of medicinal plant leaf extracts against pathogenic bacteria. *Asian Pacific Journal of Tropical Disease*, *4*, S920-S923.
6. Nascimento, G. G., Locatelli, J., Freitas, P. C., & Silva, G. L. (2000). Antibacterial activity of plant extracts and phytochemicals on antibiotic-resistant bacteria. *Brazilian journal of microbiology*, *31*(4), 247-256.
7. Mahwasane, S. T., Middleton, L., & Boaduo, N. (2013). An ethnobotanical survey of indigenous knowledge on medicinal plants used by the traditional healers of the Lwamondo area, Limpopo province, South Africa. *South African Journal of Botany*, *88*, 69-75.
8. Miara, M. D., Bendif, H., Ouabed, A., Rebbas, K., Hammou, M. A., Amirat, M., ... & Teixidor-Toneu, I. (2019). Ethnoveterinary remedies used in the Algerian steppe: Exploring the relationship with traditional human herbal medicine. *Journal of ethnopharmacology*, *244*, 112164.
9. Mathur, A., Bhat, R., Prasad, G. B. K. S., Dua, V. K., Verma, S. K., & Agarwal, P. K. (2010). Antimicrobial activity of plants traditionally used as medicines against some pathogens. *Rasayan Journal of Chemistry*, *3*(4), 615-620.
10. Koleva, V., Dragoeva, A., Nanova, Z., Koynova, T., & Dashev, G. (2015). An ethnobotanical study on current status of some medicinal plants used in Bulgaria. *Int. J. Curr. Microbiol. App. Sci*, *4*(4), 297-305.
11. Hong, L., Guo, Z., Huang, K., Wei, S., Liu, B., Meng, S., & Long, C. (2015). Ethnobotanical study on medicinal plants used by Maonan people in China. *Journal of ethnobiology and ethnomedicine*, *11*(1), 32.

12. Macía, M. J., García, E., & Vidaurre, P. J. (2005). An ethnobotanical survey of medicinal plants commercialized in the markets of La Paz and El Alto, Bolivia. *Journal of ethnopharmacology*, *97*(2), 337-350.
13. Tsioutsiou, E. E., Giordani, P., Hanlidou, E., Biagi, M., De Feo, V., & Cornara, L. (2019). Ethnobotanical study of medicinal plants used in central Macedonia, Greece. *Evidence-Based Complementary and Alternative Medicine*, *2019*.
14. Shah, N. C. (1987). Ethnobotany in the Mountainous region of Kumaon Himalaya. *Thesis submitted to the Kumaon Univ. Nainital for PhD in Botany*, 83-85.
15. Santhosh Kumar, P., Tambhekar, N., & Nayak, S. U. (2014). Ethnobotanical survey of drugs used in south India for respiratory disorders. The Journal of Ethnobiology and Traditional Medicine, 121, 787-792.
16. Saranraj, P., Bhavani, L., & Suganthi, K. (2016). Ethnobotanical survey of medicinal plants from Vellore district, Tamil nadu, India. *Int. J. Adv. Res. Biol. Sci*, *3*(9), 238-246.
17. Chakraborty, R., De, B., Devanna, N., & Sen, S. (2012). North-East India an ethnic storehouse of unexplored medicinal plants. *J Nat Prod Plant Resour*, *2*(1), 143-152.
18. Panigrahy, J., Behera, S. K., Venugopal, A., & Leelaveni, A. (2016). Ethnomedicinal study of some medicinal plants from Kandhamal district, Odisha. *Int. J. Herbal Med*, *4*(5), 36-40.
19. Smita, R., Sangeeta, R., Kumar, S. S., Soumya, S., & Deepak, P. (2012). An ethnobotanical survey of medicinal plants in Semiliguda of Koraput District, Odisha, India. *Research Journal of Recent Sciences*, *2*(8), 20-30.
20. Kumar, M., Butt, T. A., Hussaini, S.A., Kumar, K., Khan, H., Aminuddin & Samiulla, L. (2014) Ethnomedicines in the Khordha forest division of Khordha district, Odisha, India. International Journal of Current microbiology and applied sciences, 3(1), 274-280.
21. Prusti, A. B., & Behera, K. K. (2007). Ethnobotanical exploration of Malkangiri district of Orissa, India. *Ethnobotanical Leaflets*, *2007*(1), 14.
22. Biswas, S., Sahu, D. K., Dhal, N. K., & Brahmam, M. (2009). Ethnobotany of Gadaba tribe of Malkangiri district, Orissa, India. *Journal of Economic and Taxonomic Botany*, *33*(4), 910-914.
23. Dhal, N. K., Panda, S. S., & Muduli, S. D. (2014). Ethnobotanical Studies in Nawarangpur District, Odisha, India. *Am. J. Phytomed. Clin. Therapeu*, *2*(2), 257-276.
24. Sahu, S. C., Pattnaik, S. K., Sahoo, S. L., Lenka, S. S., & Dhal, N. K. (2011). Ethnobotanical study of medicinal plants in the coastal districts of Odisha. *Current Botany*.
25. Singh, H., Krishna, G., & Baske, P. K. (2010). Plants used in the treatment of joint diseases (rheumatism, arthritis, gout and lumbago) in Mayurbhanj district of Odisha, India. *Report and opinion*, *2*(9), 22-26.
26. Manandhar, S., Luitel, S., & Dahal, R. K. (2019). In Vitro Antimicrobial activity of some medicinal plants against human pathogenic bacteria. *Journal of tropical medicine*, *2019*.
27. Thatoi, H. N., Panda, S. K., Rath, S. K., & Dutta, S. K. (2008). Antimicrobial activity and ethnomedicinal uses of some medicinal plants from Similipal Biosphere Reserve, Orissa. *Asian Journal of Plant Sciences*, *7*(3), 260-267.
28. Mahalik, G., Satapathy, K. B., & Sahoo, S. (2015). Ethnobotanical survey of plants used in treatment of urinary disorders in Dhenkanal district of Odisha, India. *Journal of Environmental Science, Toxicology and Food Technology*, *9*(8), 58-63.
29. Mishra, J., Mahalik, G., & Parida, S. (2019). Ethnobotanical study of traditional medicinal plants used in the management of diabetes in the urban areas of Khurda, Odisha, India. *Asian J Pharm Clin Res*, *12*(9), 73-78.
30. Dash, G., Mohanty, K. K. G. R., Sahoo, D., Mahalik, G., & Parida, S. (2018). Traditional medicinal plants used for the treatment of asthma in Bhubaneswar, Odisha. *Int J Herb Med*, *6*(5), 57-60.
31. Manandhar, S., Luitel, S., & Dahal, R. K. (2019). In Vitro Antimicrobial activity of some medicinal plants against human pathogenic bacteria. *Journal of tropical medicine*, *2019*.
32. Egamberdieva, D., Wirth, S., Behrendt, U., Ahmad, P., & Berg, G. (2017). Antimicrobial activity of medicinal plants correlates with the proportion of antagonistic endophytes. *Frontiers in microbiology*, *8*, 199.
33. Dabur, R., Gupta, A., Mandal, T. K., Singh, D. D., Bajpai, V., Gurav, A. M., & Lavekar, G. S. (2007). Antimicrobial activity of some Indian medicinal plants. *African Journal of Traditional, Complementary and Alternative Medicines*, *4*(3), 313-318.
34. Rios, J. L., & Recio, M. C. (2005). Medicinal plants and antimicrobial activity. *Journal of ethnopharmacology*, *100*(1-2), 80-84.

35. Salhi, N., Saghir, M., Ayesh, S., Terzi, V., Brahmi, I., Ghedairi, N., & Bissati, S. (2017). Antifungal activity of aqueous extracts of some dominant Algerian medicinal plants. *BioMed research international*, *2017*.

Table.1. List of entobotanical plants and their uses (26-30, 19)

Sl. No.	Local name	Botanical name	Family	Plant part use	Cure diseases
1	Bacha	*Acorus calamus* L.	Aracaceae	Rhizome	Promotion of memory power, worm infection
2	Gheekumari	*Aloe vera* L.	Asphodelaceae	Leaf pulp,root	Madness, stomach disorder, mastitis, burnt skin and wound
3	Odosomari	*Argemone mexicana* L.	Poppies	Seed, bark, leaf	Skin disease, syphilis, wound and rat bites
4	Shatavari	*Asparagus racemosus* Willd.	Asparagaceae	Whole plant	Protects pregnancy
5	Neema	*Azadirachta indica* A. Juss.	Meliaceae	Leaf, bud	Boils, small pox, leprosy, skin disease
6	Arakha	*Calotropis gigantea* L.	Asclepiadaceae	Root, latex	Cat bite, headache and twoothache
7	Bada chakuna	*Cassia occidentalis* L.	Fabaceae	Seed, root	Eczema,filarial and asthma
8	Sadabihari	Catharanthus roseus (L.) G. Don	Apocynaceae	Leaf, root	Skin disease, insect stings, diabetes
9	Thalakudi	*Centella asiatica* (L.) Urb.	Apiaceae	Leaf	Jaundice and for development of memory, I.Q and immunity
10	Akanbindhi	*Cissampelos pareira* L.	Menispermaceae	Root, stem, bark	Leprosy, migraine, haemorrhoids and dysentery
11	Hadabhanga	*Cissus quadrangularis* L.	Vitaceae	Whole plant	Bone fracture and constipation
12	Aparajita	*Clitoria ternatea* L.	Fabaceae	Leaf, flower, fruit, root	Acne, boils and filarial
13	Talamuli	*Curculigo orchioides* Gaertn.	Hypoxidaceae	Root	Promotion of colourcomplexion, sexual strength, dysuria and leucorrhoea

14	Bana haladi	*Curcuma aromatic* Salisb.	Zingiberaceae	Rhizome	Blood dysentery, stomach disorder, indigestion, kill intestinal worms
15	Haladi	*Curcuma longa* L.	Zingiberaceae	Rhizome	Boils, eczema, chicken pox, allergies and kill worms
16	Dhanwantari	*Cymbopogon martini* (Roxb.)W.Watson	Poaceae	Leaf, plant, oil	Mosquito repellent, fever, constipation, cold, cough and headache
17	Anla	*Emblica officinalis* Gaertn.	Phyllanthaceae	Fruit	Gout, dysuria, urticaria, hair loss and dandruff
18	Khirakanchana	*Euphorbia fusiformis* Buch.	Euphorbiaceae	Dry plant root	Skin diseases and milk deficiency
19	Khadisiju	*Euphorbia tirucalli* L.	Ephorbiaceae	Latex, root	Toothache and stomach-ache
20	Bara	*Ficus benghalensis* L.	Moraceae	Bark, leaf	Mouth infection, skin disease and diarrhea
21	Sugandi	*Hemidesmus indicus* R.Br.	Apocynaceae	Root	Syphilis and piles
22	Mandara	*Hibiscus rosa-sinensis* L.	Malvaceae	Flower, leaf	Growth of air and skin diseases
23	Manjuati	*Lawsonia inermis* L.	Lythraceae	Root, leaf	Jaundice and hair loss
24	Mahula	*Madhuca indica* J.F.Gmel.	Sapotaceae	Flower, root	Impotency and snake bite
25	Nageswara	*Mesua ferrae* L.	Calophyllaceae	Flower	Leucorrhoea, menorrhagia and haemorrhoids
26	Lajakuli	*Mimosa pudica* L.	Mimosaceae	Leaf, root	Eczema, piles and toothache
27	Mersinga	*Murraya koenigii* L.	Rutaceae	Leaf	Belching and hair loss
28	Durlava	*Ocimum basilicum* L.	Lamiaceae	Leaf, seed	Dysuria, cough and cold
29	Tulasi	*Ocimum sanctum* L.	Lamiaceae	Leaf, seed	Waist pain, blood dysentery and headache

30	Posaruni	*Paederia foetida* L.	Rubiaceae	Leaf	Nyctalopia, stomach pain during menstrual cycle, cough and cold
31	Gol maricha	*Piper nigrum* L.	Piperaceae	Fruit	Leucorrhoea and alati
32	Badianla	*Phyllanthus niruri* Hook. F.	Phyllanthaceae	Whole plant	Diabetes, prevention of malaria and skin diseases
33	Karanja	*Pongamia pinnata* L.	Papilionaceae	Leaves	Headache, diarrhea, burns and wounds
34	Rakta Chandan	*Pterocarpus santalinus* L.f.	Fabaceae	Bark, shoot	Fever, corneal capacity, high blood pressure and diabetes
35	Patalagaruda	*Rauvolfia serpentine* Benth.ex. Kurz	Apocynaceae	Whole plant, leaf, rhizome	Irregular menstruation, gum bleeding, dysuria and calculus
36	Asoka	*Saraca asoca* (Roxb.)Wild.	Fabaceae	Bark, seed, flower	Measles, relieve pain from fractured spot
37	Sal	*Shorea robusta* Gaerthn.f.	Dipterocarpaceae	Bark, leaves	Spermatorrhea and acne
38	Arjuna	*Terminalia arjuna* Roxb.	Combretaceae	Whole plant	Acne
39	Bisalyakarani	*Tridax procumbens* L.	Asteraceae	Leaf	Cuts and wounds
40	Ada	*Zingiber officinale* L.	Zingiberaceae	rhizome	Vomiting, nausea, cold and indigestion
41	Basanga	*Justicia adhatoda* L.	Acanthaceae	bark	Stomach pain
42	Pokasungha	*Ageratum conyzoides* L.	Compositae	leaf	Scabies
43	Panasa	*Artocarpus heterophyllus* Lam.	Moraceae	root	Lactation in expectant mother
44	Agara	*Argemone mexicana* L.	Papaveraceae	latex	Rheumatic pain, infection of eye
45	Sorisa	*Brassica juncea* (L.) Czern.	Cruciferae	seed	Skin disease, cold
46	Salapa	*Caryota urens* L.	Palmaceae	root	To get relieved from the effect caused due to

					intake of salapa in case of pregnant women.
47	Lembu	*Citrus medica* L.	Rutaceae	fruit	Boil, Vomiting
48	Saru	Colocasia esculenta (L.) Schott	Araceae	tuber	Boil
49	Kalachakunda	*Cassia occidentalis* L.	Caesalpiniaceae	leaf	wound
50	Phutaphutika	*Cardiospermum halicacabum* L.	Sapindaceae	tuber	Joint pain
51	Kapa	*Gossypium hirsutum* L.	Malvaceae	Root and fruit	Cough
52	Banatulsi	*Ocimum canum* L.	Labiatae	leaf	Migraine
53	Jada	*Ricinus communis* L.	Euphorbiaceae	seed	Pain in hands, legs and head
54	Sapua	*Sansevieria roxburghiana* Schult. & Schult.f.	Liliaceae	Juice	Burns
55	Bhejri	*Solanum xanthocarpum* Schrad & Wendl	Solanaceae	fruit	Toothache
56	Tentuli	*Tamarindus indica* L.	Caesalpiniaceae	Fruit, tender leaf	Constipation, round worm
57	Banaphula	*Mirabilis jalapa* L.	Nyctaginaceae	Tuberous root	Fever, stomach pain
58	Karabira	*Nerium oleander* L.	Apocynaceae	bark	Blood in stool
59	Katha champa	*Plumeria rubra* L.	Apocynaceae	Bark, flower	Cold and cough
60	Dalimba	*Punicum granatum* L.	Onagraceae	Tender fruit	Dysentery
61	Banakolatha	*Atylosia scarabaeoides* (L.) Benth.	Papilionaceae	root	Fids
62	Brudhajarak	*Argyreai speciosa* (Linn.f.) sweet	Convolvulaceae	root	Weakness
63	Banahaladi	*Curcuma aromatic* Salisb.	Zingiberaceae	tuber	Burning of stomach
64	Kendriphala	*Chenopodium ambrosioides* L.	Chenopodiaceae	stem	To get rid of evil sprit
65	Khadisiju	*Euphorbia tirucalli* L.	Euphorbiaceae	leaf	Waist pain
66	Sajana	*Moringa oleifera* Lam.	Moringaceae	leaf	Cold
67	Agasti	*Sesbania grandiflora* (L.)Pers.	Papilionaceae	Fruit, leaf	Fever, night blindness
68	Akanabindi	*Stephania hernandifolia* (Willd.) Walp.	Menispermaceae	root	Fever, diahorrea
69	Mayurschulia	*Elephantopus scaber* L.	Asteraceae	Stem	Fever
70	Dhuanpatra	*Nicotiana tabacum* L.	Solanaceae	leaf	Snake bite
71	Nilgiri	*Eucalyptus globules* Labill.	Myrtaceae	leaf	Constipation, bird lice
72	Jamokoli	*Eugenia jambolana* Lam.	Myrtaceae	bark	Blood dysentery
73	Pijuli	*Psidium guajava* L.	Myrtaceae	Bark, fruit	Dysentery, blood dysentery
74	Lalkhada	*Amaranthus tricolor* L.	Amaranthaceae	leaf	anemia
75	kalara	Momordica charantia	Cucurbitaceae	leaf	Earache, ringworm
76	Amrutabhanda	*Carica papaya* L.	Passifloraceae	fruit	Lactation

77	Dadura	*Datura stramonium* L.	Solanaceae	Flower and leaves	Asthma
78	Manjuati	*Lawsonia inermis* L.	Lythraceae	root	Jaundice
79	Aamba	*Mangifera indica* L.	Anacardiaceae	Bark, Kernel	Diarrhea, bleeding of nose
80	Piaja	*Allium cepa* L.	Liliaceae	bulb	Cough and cold
81	pedipedica	*Abutilon indicum* (L.) Sweet	Malvaceae	root	Jaundice, piles
82	Apamaranga	*Achyranthes aspera* L.	Amaranthaceae	bark	Sprain, dysentery, constipation
83	Chhatiana	*Alstonia scholaris* (L.) R. Br.	Apocyanceae	leaf	Lice
84	Bhuinnimba	*Andrographis paniculata* (Burm.f.) Wall. Ex Nees	Acanthaceae	Whole plant, leaf, root	Skin disease, malaria, stomach pain, dysentery
85	Iswarmula	*Aristolochia indica* L.	Aristolochiaceae	leaf	Snakebite
86	Brahmi	*Bacopa monnieri* (L.) Rennell	Scrophulariaceae	Whole plant	Increase of memory power
87	Daskerenta	*Barleria prionitis* L.	Acanthaceae	Leaf	Cuts, wounds, malaria
88	Hemsagar	Bryophyllumcalycinasalisb.	Crassulaceae	Leaf	Burns, diarrhea
89	Palasi	*Butea monosperma* (Lam.) Taub.	Fabaceae	seed	Diarrhea
90	Dhanualanka	*Capsicum frutescens* L.	Solanaceae	Fruit	Waist pain
91	Kumbhi	*Careya arborea* Roxb.	Barringtoniaceae	Bark	Diarrhea
92	Agnijhal	*Clausena excavate* Burm.f.	Rutaceae	Root	Loss of appetite
93	Kunduri	*Coccinia grandis*	Cucurbitaceae	Fruit	Stomach pain of children, filaria swelling
94	Dahadahia	*Coculus hirsutus* (L.) Diels	Menispermaceae	Leaf, root	Spermatorrhea& leucorrhoea, stomach pain
95	Nirmuli	*Cuscutare flexa* Roxb.	Convolvulacea	Stem	Fever, malaria
96	Mansa siju	*Euphorbia antiquorum* L.	Euphorbiaceae	Whole plant	Cough & cold
97	Dimiri	*Ficus racemose* L.	Moraceae	Fruit	Headache
98	Kuduchi	*Holarrhena pubescens* wall.	Apocynaceae	Bark, root, seed	Blood dysentery, stomach pain
99	Koilirekha	*Hygrophila auriculate* (K.Schum.) Heine.	Acanthaceae	Leaf	Cough
100	Baula	*Mimusops elengi* L.	Sapotaceae	fruit	Loose teeth

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RESEARCH ARTICLE

Comparative Study on Financial Performance of Hindustan Unilever and Nestle India

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ABSTRACT

In present uncertain environments, measuring the financial performance as well as financial position is most significant for corporate sector in the field of manufacturing. The study of financial performance replicates the financial position as well as profitability of the corporate sector is vital as there are neck and neck competitions in the same business. As the comprehensive data about the financial performance and position accessible for all therefore the manager, investors, and creditors can put on the different financial strategy by financial analysing their tactical thinking in the investment decisions. Accordingly, this research comprises the financial performance of two major firm sin consumer and non-durables manufacturing companies in India i.e. Hindustan Unilever Ltd. and Nestle India Ltd. To examine the financial performance of Hindustan Unilever Ltd. and Nestle India Ltd. data has been composed from the data published from different website for the ten years from 2009-10 to 2018-19. Different financial ratios and t test have been applied to study the financial performance of Hindustan Unilever Ltd. and Nestle India Ltd.

Keywords: Financial Performance, Financial Ratios; Current Ratio, Inventory Turnover Ratio, Net Profit Margin and Return on Total Assets.

INTRODUCTION

Now a day's all over the world companies are not only concern about their sales but also they want more productivity, management style, skilled manpower, increased quality of the products, good service quality and

marketing. Competition is very high in the global market, so all the corporates have to be ready to meet the challenges. So analyzing financial performance of the company is the measure task to follow. Financial performance of the company is the key issue in every company. Finance is the provision of money and resources at the time of requirement. Financial management is concerned about the arrangement and so also utilization of funds in a company. Finance managers have to plan and control the financial resources. They have to take number of decisions in a company by using different financial management techniques. The final results of the proper decisions will be found in profit and loss account and balance sheet of the corporates. Profit and loss account gives the profit and loss of a business for a particular period of time whereas balance sheet shows the financial position of business for a point of time. Financial Performance analysis is mainly concerned with the analysis of profit and loss account and balance sheet of a company. Financial statement analysis, financial ratio analysis are the common techniques which are used to measure the financial performance of a company. Different financial ratios are used to know the financial health of a company. Short term liquidity position and also long term financial position can be analysed through the help of different financial ratios. Financial ratios are very much helpful to know how effectively the company is using its assets to get profit, how efficiently the organization is operating its business, how the company is managing its debt. It shows whether the company will be sustainable in long run or not. It explains whether the company is able to satisfy the stakeholders or not. It gives the overall financial performance of the company.

LITERATURE REVIEW

Deloof (2003) Investigated that big companies are investing huge amount of money in the working capital. So it is very important to manage the working capital of the company as it will affect the financial performance of the companies. He has used correlation and regression analysis for the study. He found that there is a negative correlation between gross operating income and bills receivable, bills payable and inventories of the companies. While Dheenadayalan and Deviananbrasi4 (2007) have found Z score of their sample companies. They have studied for a period of 1997 to 2007. They found that the company's financial position was not good, they are also facing insolvency. On the other hand Boubacar (2011) have done their studies to find whether the foreign Bank subsidiaries financial performance is good or not. They found that the ownership is generally with the parent bank. Similarly Srinvas(2010) has studied the financial performance of different banks after and before merger in India. He has taken six banks for his study. He found that private banks financial performance is better than the public sector bank after merger. Whereas Bhatasna and Raiyani (2011) have investigated the financial position of Textile Industries in India.They have taken Z score method for their analysis. They found that some of the selected companies are financially good throughout the study period. But in some company Z score is lower. Additional Paul (2011) investigated to find the financial performance of NBFCs. He has done the comparative study of NBFCs. He found a sound financial health of the selected companies for the particular period. Similarly, Patjoshi (2016) in his study involves the financial performance of two major companies i.e. HINDALCO and NALCO aluminium manufacturing companies in India. To analyze financial performance of HINDALCO and NALCO data has been self-possessed from the data published from different website for the ten years from 2005-06 to 2014-15. Different financial ratios and t test have been employed to study the financial performance of HINDALCO and NALCO.

Brief Profile of Nestle India Ltd.

Nestle started its business in India in 1961, in Moga, Punjab. Now it is with four offices and eight production units in India. Nestle is very closely associated with India, and satisfying its stakeholder. The company is giving large number of employment opportunities to the Indian people. Nearly one million people are getting benefit from the employment. The quality of the company's product is famous in both national and international market. The famous brands of the compny are Nescafé, Maggi, Milkybar, Kit Kat, Bar-One, Milkmaid and Nestea.

Brief Profile of Hindustan Unilever Ltd.

Hindustan Unilever Ltd (HUL) started its business in 1993 in India. It is one of the biggest fast moving consumer goods (FMCG) corporations in India. HUL is earning very high amount of profit in the competitive market where

large numbers of competitors are entering to the market. They are achieving their target through innovations, marketing and efficient management. Their research and development is helping them to apply innovations in the product and marketing. The company is in the 12th position in the super 50 list of the world's most innovative companies in the financial year 2012-13, by Forbes.

18 brands of the company are in the '100 Most Trusted Brands' list by Brand Equity. HUL mostly files 250 to 350 new patent applications in a year. The company has over 20,000 registered patents and patent applications all over the world.

Objectives of the Study

The following are the detailed objectives of the study.

1. To analyze the financial performance as well as financial position of Hindustan Unilever and Nestle Indiafrom 2009-10 to 2018-19.
2. To study the comparative liquidity and profitability position ofHindustan Unilever and Nestle Indiafrom 2009-10 to 2018-19.

Hypothesis of the Study

Keeping the objectives in view, the hypothesis framed for the study is

Ho: There is no significant difference between different financial ratios of Hindustan Unilever and Nestle India.

METHODOLOGY OF THE STUDY

To analyze financial performance of Hindustan Unilever andNestle India data has been collected and poised from the data published different website for the ten years from 2009-10 to 2018-19. The collected data have been suitably re-arranged, classified and tabulated as per the requirements of the study. Different financial ratios and t test have been employed to study the financial performance of Hindustan Unilever and Nestle India. To study financial performance of Hindustan Unilever and Nestle India different financial ratios like Current Ratio (CR), Inventory Turnover Ratio (ITR), Net Profit Margin (NPM) and Return on Total Assets (ROTA) have been calculated. The t test has been employed for the testing of hypothesis.

DATA ANALYSIS AND DISCUSSION

Analysis of Major Financial Ratio

The analysis of major financial ratios alike Current Ratio (CR), Inventory Turnover Ratio (ITR), Net Profit Margin (NPM) and Return on Total Assets (ROTA) of both the companies Hindustan Unilever &Nestle India have explained in Table 1.Current Ratio measures the liquidity position of an organisation. Current Ratio is the relationamong of current assets and current liabilities. It shows the competenceto meet the current obligation of an organisation. Anappraisal on the table-1 discloses that current ratio of both companies has exposed a substantial variation during the study period. The absolute figure of current ratio of Hindustan Unilever has an average of 0.86 and varies from 0.74 to 1.43.On the other hand the current ratio ofNestle India has recorded an average of 0.59 and varies from 0.50 to 0.68. The table indicates Hindustan Unilever recorded better liquidity position as compare to Nestle India. The standard current ratio should 2:1 for an organisation. Consequently both the companies have low liquidity and fail to maintain the standard of current ratio (liquidity positions)over the study period from 2009-10 to 2018-19.

Inventory turnover ratio is the association among sales and inventory. Inventory turnover ratio displays how well the organisation manages its inventory and how many times inventory transformed into sales in anaccounting period. Inventory should uphold at a proper level, which stabilities production process and sales prerequisite. A higher inventory turnover ratio is a good sign and indicateslesser inventory holding period. From the above it found

that the inventory turnover ratios of Hindustan Unilever shows an increasing trend by recorded minimum of 7.34 times and maximum 15.78 times. On the contrary the inventory turnover ratios of Nestle India show a decreasing trend by recorded minimum of 9.64 times and maximum 12.80 times. The averages inventory turnover ratios are 11.82 times and 11.23 times for Hindustan Unileverand Nestle India respectively. As per Indian Manufacturing Companies the average inventory turnover ratio should 2.12 times. From the above both the companies have maintained higher inventory turnover ratios as compare to standard inventory turnover ratio during the study period. Accordingly, it presentedeffective management of inventory by both the companies during mentioned period.Hindustan Unilever can able to manage inventory better than Nestle India over the period of study.

Net Profit Margin furnishes a relationship between Net Profit (Profit after Tax) & Sales and designates the completeproficiency of the management in manufacturing, selling, administrative and other activities of the firm. The table-1 reveals that net profit margin Hindustan Unilever has shown an increasing trend and fluctuated from 11.68% to 15.79% during study period, whereas the net profit margin of Nestle India has fallen down from 13.07% in 2009-10to 6.88% in 2014-15 and then increased to 15.89% in the year 2018-19. The average net profit margin of Hindustan Unileverand Nestle India are 13.71% and 12.22% respectively which proposes Hindustan Unilever has performed better thanNestle India for the study period.

Return on total assets is mostsignificant ratio used for evaluating the overall efficiency of the firms, by way of the objective of firms is to make the most of its earnings. It can find from the table-1 that both the companies return on total assetshave shown an increasing trend for during the study period. The absolutepercentage of this ratio fluctuates between 11.84% and 35.27% for Hindustan Unilever. Correspondingly, return on total assets of Nestle India has fluctuates between 88.72% and 381.03%. But it can also perceive that in all the years of study there is a wide gap in returns on total assets between the Hindustan Unilever and Nestle India. The average returns on total assets are 21.21% and 248.84%, which proposesNestle India has performed better than Hindustan Unilever.As a result, the returns on total assets of the both the companies are satisfactory during the period under study.

Analysist-Test: Paired Two Sample of Current Ratios

Table 2 reviews the results of current ratios of Hindustan Unilever along withNestle Indiafrom 2009-10 to 2018-19through the assistance of t-test. The t-test consequence for the current ratio indicates that mean current ratio of Hindustan Unileveris more as compared to that of the Nestle India; leading to the decision that liquidity position of Hindustan Unileveris better. In contrast, lower variance for Nestle India current ratio as compared to Hindustan Unilevercurrent ratio clearly designates that former is more consistent than the latter. Nevertheless, the correlation value is 0.17 represents positive correlation of current ratio among both the companies during study period. The p-value of 0.00, which is less than 0.01, specifies a significant difference in the value of current ratio between Hindustan Unilever and Nestle Indiaat 1 percent level of significance.

Analysist-Test: Paired Two Sample of Inventory Turnover Ratios

The above table evidently displays that mean value of inventory turnover ratio is higher of Hindustan Unileveras compared to Nestle India over the period of study, describes the better inventory management applies of Hindustan Unilever. On the other hand the inventory turnover ratio of Hindustan Unileverhas shown more variation than that of Nestle India, as variance shows higher value of Hindustan Unileverthan that of Nestle India. The correlation value of inventory turnover ratios of both companies is -0.38 denotesnegative correlation between both the companies. The p-value of 0.30in case of inventory turnover ratio point towardno significant difference between the inventory turnover ratios of both the companies.

Analysist-Test: Paired Two Sample of Net Profit Margin

The mean of net profit margin is higher in case of Hindustan Unileveras compared to Nestle India. The variation of Hindustan Unilevernet profit margin is less than the Nestle Indianet profit margin as variance is found to be less in

Hindustan Unilever for the study period. As the correlation is 0.23 which indicates that there is a positive correlation present between net profit margin of Hindustan Unilever and Nestle India. At this juncture too there is no significant difference between Hindustan Unilever and Nestle India net profit margin as the p-value is 0.05.

Analysist-Test: Paired Two Sample of Return on Total Assets

From the table 5, it is demonstrated that return on total assets has not shown the similar trend like that of net profit margin. The mean value and the variance of return on total assets of Nestle India are found much higher than that of Hindustan Unilever. Consequently there is less consistency in case of Nestle India return on total assets. The correlation value of 0.58 suggests returns on total assets of both companies are highly positive correlatedpresent between return on total assets of Hindustan Unilever and Nestle India. The p value proves that there is a significant difference between Hindustan Unilever and Nestle India return on total assets among the two companies for the study period.

CONCLUSION

This research is associated to the comparative financial performance of Hindustan Unilever and Nestle India over ten years from 2009-10 to 2018-19. Interpretation to succeeding evaluation, it can be determined that during the study period the complete performance in relations to profitability and liquidity position have varied significantly for both the companies. Hindustan Unilever recorded better liquidity position as compare to Nestle India but both the companies have maintained low liquidity position and fail to maintain the standard of current ratio (liquidity positions) over the study period. In contrast both the companies presented effective management of inventory during mentioned period while Hindustan Unilever can able to manage inventory better than Nestle India over the period of study. In the case of net profit margin Hindustan Unilever has performed better thanNestle India for the study period. Nonetheless in the case of return on total assets Nestle India has performed far better than Hindustan Unilever.It can observe from the t test that there is significant difference between current ratio and return on total assets of Hindustan Unilever and Nestle India. Therefore the null hypothesis (there is no significant difference between different financial ratios of Hindustan Unilever and Nestle India) is rejected and alternative hypothesis is accepted in the case of current ratio and return on total assets. While the inventory turnover ratio and net profit margin has shown no significant difference.Consequently the null hypothesis (there is no significant difference between different financial ratios of Hindustan Unilever and Nestle India) is accepted and alternative hypothesis is rejected for inventory turnover ratio and net profit margin.

REFERENCES

1. Bhatasna, P.B. andRaiyani,J. R. (2011). "A Study on Financial Health of Textile Industry in India: A 'Z' – Score Approach" Indian Journal of Finance, Vol.5, No.1 p.9-16..
2. Chundawat, D.S. and Bhanawat, S.S. (2000)."Working Capital Management Practices in IDBI assisted Tube and Tyre Companies", The Management Accountant, Vol 35, no 2, pp.99-102.
3. Deloof. M. (2003). "Does working capital management affects profitability of firms" vol 30 no 3 pp.33-43.
4. Dheenadayalan V and Devianabrasi, R.(2007). "Financial Health of Cooperative Sugar Mill a Case Study of NPKRR Cooperative Sugar Mills Ltd., Indian Co-operative Review, vol 7 no 3 pp.192-197.
5. Boubacar, H. (2011). "The Financial Performance of Foreign Bank Subsidiaries" Indian Journal of Finance, Vol.5, No.1, p.3-8.
6. Patjoshi, P. (2016). "A Comparative Study on Financial Performance of HINDLCO and NALCO" International Journal of Business Environment, 5(3),:2373-2379.
7. Paul, P. (2011). "Financial Performance Evaluation- A comparative Study of some Selected NBFCs "Indian Journal of Finance, Vol. 5 No.5 p.13-22'

8. Shiralashetti, A.S. (2011). Performance Appraisal of the GADAG Co-Operative Cotton Textile Mill Ltd, HULKOTI – A Case Study" SMART Journal of Business Management Studies, Vol.7, No.1, p.13-21
9. Srinivas, K. (2010). 'Pre and Post Merger financial performance of merged Banks in India' Indian Journal of Finance, Vol.4, No.1, p.3-19.
10. Velavan, M.(2010).."Measuring Financial Health of E.I.D. Parry Sugar Ltd Using 'Z' Scaore Model- A Case Study" Indian Journal of Finance, Vol. 4, No.11 p.30-43.

Table 1: Trend of Major Financial Ratio of Hindustan Unilever &Nestle India

Year	Current Ratio		Inventory Turnover Ratio		Net Profit Margin (%)		Return on Total Assets (%)	
	Hindustan Unilever	Nestle India	Hindustan Unilever	Nestle India	Hindustan Unilever	Nestle India	Hindustan Unilever	Nestle India
2009-10	0.84	0.62	8.99	12.33	12.39	13.07	11.84	88.72
2010-11	0.86	0.55	7.34	10.49	11.68	12.79	12.31	132.13
2011-12	0.83	0.54	9.21	11.55	12.16	12.81	16.25	186.53
2012-13	0.76	0.65	10.80	12.80	14.70	12.27	12.36	245.68
2013-14	0.74	0.53	10.76	12.06	13.80	12.02	15.15	294.27
2014-15	0.75	0.50	12.57	10.33	14.00	6.88	17.21	292.26
2015-16	1.03	0.57	13.25	10.13	13.31	10.04	29.02	312.57
2016-17	0.82	0.68	14.60	11.29	14.07	12.24	29.99	354.78
2017-18	0.94	0.67	14.93	11.70	15.16	14.23	32.69	381.03
2018-19	1.00	0.58	15.78	9.64	15.79	15.89	35.27	200.40
Average	0.86	0.59	11.82	11.23	13.71	12.22	21.21	248.84
Minimum	0.74	0.50	7.34	9.64	11.68	6.88	11.84	88.72
Maximum	1.03	0.68	15.78	12.80	15.79	15.89	35.27	381.03

Table 2: t-Test: Paired Two Sample of Current Ratio

Particulars	Hindustan Unilever	Nestle India
Mean	0.86	0.59
Variance	0.01	0.00
Pearson Correlation	0.17	
t Stat	7.68	
P(T<=t) one-tail	0.00	
t Critical one-tail	1.83	
P(T<=t) two-tail	0.00	
t Critical two-tail	2.26	

Table 3: t-Test: Paired Two Sample of Inventory Turnover Ratio

Particulars	Hindustan Unilever	Nestle India
Mean	11.82	11.23
Variance	8.08	1.09
Pearson Correlation	-0.38	

t Stat	0.55	
P(T<=t) one-tail	0.30	
t Critical one-tail	1.83	
P(T<=t) two-tail	0.59	
t Critical two-tail	2.26	

Table 4: t-Test: Paired Two Sample of Net Profit Margin

Particulars	Hindustan Unilever	Nestle India
Mean	13.71	12.22
Variance	1.78	5.80
Pearson Correlation	0.23	
t Stat	1.90	
P(T<=t) one-tail	0.05	
t Critical one-tail	1.83	
P(T<=t) two-tail	0.09	
t Critical two-tail	2.26	

Table 5: t-Test: Paired Two Sample of Return on Total Assets

Particulars	Hindustan Unilever	Nestle India
Mean	21.21	248.84
Variance	87.80	9134.09
Pearson Correlation	0.58	
t Stat	-7.96	
P(T<=t) one-tail	0.00	
t Critical one-tail	1.83	
P(T<=t) two-tail	0.00	
t Critical two-tail	2.26	

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RESEARCH ARTICLE

Interrelationship between Capital Structure and Financial Efficiency: Case Study of ACC

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ABSTRACT

Capital structure is extreme notice able adjustment of organization's processes. The relations between capital structure and profitability of an organization have been received substantial thought in the financial management. Capital structure is very important part in the financial decision, as it directly related to the risk and return of an organization. Whether the capital structure of an organization has impact on the financial performance is a matter of investigation for important decision making. Therefore, this study purposes is to find out the interrelationship between Capital Structure and Financial Efficiency of ACC for a period of ten years from 2005-06 to 2014-15. The collected data has examined through the correlation and regression analysis for finding out the interrelationship between capital structure and financial efficiency of ACC. Correlation analysis has used for finding out the connection between capital structure and financial efficiency. The study has considered the secondary data for the period. The different financial ratios (capital structure ratios and profitability ratios) have been used for the investigation.

Keywords: Capital Structure, Financial Performance; Debt Equity Ratio and Profitability Ratios.

INTRODUCTION

Financial structure is the combination of all liabilities (both short term as well as long term) whereas Capital structure is the combination of only long-term liabilities an organization. Hence Capital structure is the combination of an organization's common share capital, preferred share capital, long-term debt and retained earnings, which

have been used to finance its general practices and development. Capital structure is a genuine important financial decision as it directly associated to the risk and return of an organization. Any in appropriate combination of capital structure decision can be resulted in high cost of capital; thus the organization's value will suffer though inappropriate capital structure decision Optimum capital structure is that capital structure which leads to the maximum value of the firm and minimize the organization's cost of capital. More or less, different researchers have different view and use to defined capital structure in their personal manner. The capital structure has derived by Weston and Brigham (1979) as the permanent financing of a firm signified by long-term debt, preferred stock and shareholders' funds. Van Horne and Wachowicz(1995), defined capital structure is the mix of a firm's permanent long-term financing represented by debt, preferred stock, and common stock equity. Therefore, it can be imitative that capital structure syndicates mainly equity and long-term debt. If an organization financed by means of debt or borrowed funds then it has to pay the interest to the money lender and if it financed by equity, it has to distribute some part of profits as dividends to the share holders. In the other hand organization keeps its undistributed profit as retained profit in reverses and surplus, which is a part of shareholders' funds. The interrelationship between capital structure and profitability or financial efficiency of the organization is very important part that received substantial consideration in the financial management. An organization's profitability use to measure by maximizing the shareholders' funds is at the end of a period as compare to at the beginning the period. The main objective of shareholders from the business is to increase wealth from the investments. Thus the dimension of financial performance of the organization must provide a sign in the way to maximize shareholder wealth which will consequence in the investment over a specific time. It is clear from the above conversation; one significant thing is understandable that the capital structure has great influence on organization's profitability. Therefore, this study purposes is to find out the interrelationship between capital structure and financial efficiency of ACC from2005-06 to 2014-15.

Brief Profile of ACC

ACC Limited is India's leading manufacturer of cement and ready mixed concrete with 17 contemporary cement factories, more than 50 ready mixed concrete plants, and a vast circulation network of over 9,000 dealers and a nation wide range of sales distributors. ACC has been an innovator and well-known brand in cement and concrete technology. ACC was established in 1936 and has an exceptional track record of advanced research, product expansion and expert consultancy services. ACC is identical with cement and appreciates a high level of equity in the Indian financial market. Therefore ACC is a principal brand from last eight decades having un appalled merge with a vision to attend customers, stakeholders and the nation with commitment. Today ACC represents not only a trademark in cement as well as in concrete but also a brand name which reposes on many potentials in high quality building materials, great place to work, reliable business associates and good corporate citizen.

LITERATURE REVIEW

Gleason, Lynette, and Ike (2000) found from their research that high debt in the capital structure would decrease the firm's profitability. They experienced that firm's capital structure has a statistically negative result onfirm's profitability matrixes. Similarly observed by Fama and French(2002), they identified that extremely profitable companies with lesser risk of financial suffering are really less levered which challenges through the trade-off model. Manawaduge, Zoysa, Chowdhury, and Chandarakumara (2011) determined that most of the Sri Lankan companies' use short-term debt as in contradiction of the long-term debt and firm profitability is negatively affected by the use of debt. Similar Khairul (2013) observed remarkable negative association amongst performance and leverage in Bangladeshi companies. Tianyu (2013) inspected the effect of capital structure on firm's profitability in both industrialized and developing markets using OLS regression technique, he recognized that capital structure has a negative result on company's profitability in China, Margaritis and Psillaki (2010) in their article observed an important positive relation among capital structure and companies financial performance. In the same way Samuel

(2013) examined the connotation amongst capital structure and, although they got a negative relation among capital structure and ROA. Though, they observed no important association among ROE and capital structure.

Objectives of the Study

The attention of this study is interrelationship between capital structure and financial efficiency of ACC

1. To analyses the capital structure and profitability position of ACC
2. To measure the interrelationship between capital structure and financial efficiency of ACC.

METHODOLOGY OF THE STUDY

For fulfilling the above stated research objectives, the data for this study has been collected from the financial statements of published annual report of ACC. The collected data has investigated through the correlation, regression analysis for finding out the interrelationship between capital structure and financial efficiency of ACC, Correlation analysis has used for finding out the connection between capital structure and financial performance. The study has considered the secondary data for a period of ten years from 2005-06 to 2014-15. The different financial ratios (capital structure and profitability ratios) have been used for the investigating as follows:

A. Capital Structure Ratios: Total Debt to Equity Ratio (TDER) and Long Term Debt to Equity Ratio (LTDER)
B. Profitability Ratios: Operating Profit Margin (OPM), Net Profit Margin (NPM), Return on Capital Employed (ROCE), Return on Assets (ROA) and Return on Equity (ROE).

Data Analysis and Interpretation

Analysis of different Capital Structure Ratios of ACC

The table -1 shows the different capital structure ratios and the trend of these ratios of sample companies have elaborated below. The total debt to equity ratio (TDER) is the relationship between total debt and shareholder's funds. It is the greatest straight-forward measure of an organization's long term solvency. Normally a lower total debt to equity ratio is a sign of lower risk to the organization. On the contrary, a higher total debt to equity ratio designates higher risk to the organization or the long term solvency position of the organization is not good. Table I reveals that TDER fluctuated between 0.52 in the last year of study 2014-15 and 0.88 in the first year of study 2005-06. The average TDER of the ACC throughout the study period was 0.66, which was very low to the standard ratio of 2:1. However the ratio demonstrates a decreasing trend throughout the study period, it found to be lesser than the standard ratio of 2:1 throughout the study period. Hence, TDER is unsatisfactory all the years of study period; the company's aptitude to encounter its long-term requirements was unsatisfactory. Similarly, long term debt to equity ratio (LTDER) is also a measure of long term solvency of an organization. It is the relationship between long term debt and shareholder's funds. From the table it can find out LTDER has also shown a decreasing trend during the study period and varied between 0.07 in the year 2014-15 to 0.39 in the year 2005-06. The average LTDER of the ACC throughout the study period was 0.16. A ratio of less than one in this category indicates a higherreliance on capital provided by owners than capital providedby outsiders of the company. Therefore LTDER of ACC was found to be very low as compare to the standard ratio. Henceforth, like TDER, LTDER is also unacceptable all the years of study period; the company's ability to meet its long-term requirements was disappointing all over the study period.

Analysis of different Profitability Ratios of ACC

The table-2 revel the different Profitability ratios and theirtrend of ACC have elaborated below.Operating Profit Maegan (OPM) demonstrates firm's operating efficiency. It is the relationship between operating profit and sales. From the table it can observe that OPM shows a declining movement during the study period from 2005-06 to 2014-15. It recorded a highest of 26.03% in 2005-06 and a lowest of 7.22% in 2014-15 with an average of 18.47%. In the case of Net Profit Margin (NPM) indicates the overall efficiency of a firm. By studying the ACC's NPM, it can observe that NPM of ACC also have a decreasing trend and came down from 21.23% in the first year 2005-06 to 5.01% in the last

year 2014-15 with a mean of 14.11% for study period.Likewise OPM and NPM other profitability ratios (ROCE, ROA and ROE) of ACC have shown a diminishing trend. The ROCE, ROA and ROE of ACC have come down from 34.49%, 20.86% and 39.19% respectively to 9.43%, 4.61% and 7.01% during the study period from 2005-06 to 2014-15. These ratios have recorded average of 23.15%, 12.46% and 21.05% correspondingly for ROCE, ROA and ROE of ACC throughout the study period.

Analysis of Correlation

Correlation analysis concludes the strength and direction of the linear association among different capital structure and profitability ratios elaborated at Table 3. The correlation results of different ratios have elaborated below. Total debt to equity ratio is positively related to all profitability ratios (OPM, NPM, ROCE, ROA and ROE). It is highly correlated to ROE (0.85) and poorly correlated to ROA (0.80). Similarly long term debt to equity ratio also positively correlated to all profitability ratios. The long term debt to equity ratio has extremely correlated to ROE (0.85) and lowest correlated to OPM (0.63).

Regression Analysis Total Debt to Equity Ratio and Profitability Ratios

The below table's i.e, 4(a), (b) and (c) derived the regression analysis between TDER as dependent variable with the profitability ratios as independent variables. The goodness of fit consequences of standard linear multiple regressions through TDER as the dependent variable and numerous determinants as forecasters are described in Table 4(a), the model result has elaborated in Table 4(b). The model coefficients have revealed in Table 4(c)and the outcomes designate that no one of the indicators of TDER is significant ($p>0.05$) except ROA and ROE. This study indicates that, the association among TDER and profitability ratios by suggesting that statistically insignificant associations among TDER and on the profitability ratios except ROA and ROE. The adjusted R Square values of 0.95 designate that around 95% of the variation in TDER is clarified by the independent variables included in the model. The complete significance of the model was measured by ANOVA. The result designate that the model is statistically significant relation as demonstrated in the F value of 38.45 and a P-value < 0.01. NPM, ROCE and ROE have positive coefficient and ROE have marks the maximum influence to the forecast of the TDER with a coefficient of 5.67.While the t statistic and the Sig-values of OPM, NPM and ROCE designate insignificant associations on TDER at 5% levels. Whereas ROA and ROE have designated significant associations on TDER at 5% levels.

Regression Analysis Long Term Debt to Equity Ratio and Profitability Ratios

The below table's i.e, 5(a), (b) and (c) derived the regression analysis between TDER as dependent variable with the profitability ratios as independent variables. The goodness of fit consequences of standard linear multiple regressions through LTDER as the dependent variable and numerous determinants as forecasters are described in Table 5(a), the model result has elaborated in Table 5(b). The model coefficients have revealed in Table 5(c) and the outcomes designate that no one of the indicators of LTDER is significant ($p>0.05$) except ROE. This study indicates that, the association among LTDER and profitability ratios by suggesting that statistically insignificant associations among LTDER and on the profitability ratios except ROE. The adjusted R Square values of 0.97 designate that around 97% of the variation in LTDER is clarified by the independent variables included in the model. The complete significance of the model was measured by ANOVA. The result designate that the model is statistically significant relation as demonstrated in the F value of 25.16 and a P-value < 0.01. OPM and ROE have positive coefficient and ROE have marks the maximum influence to the forecast of the LTDER with a coefficient of 3.57.While the t statistic and the Sig-values of all profitability ratios designate insignificant associations on TDER at 5% levels except ROE.

CONCLUSION

This study is mainly related to interrelationship between capital structure and financial efficiency of ACC of ten years from 2005-06 to 2014-15. To find out the interrelationship the data has been investigated through the correlation, regression analysis. Correlation analysis has used for finding out the connection between capital

structure and financial performance whereas the relationship between the ACC's financial performance is existence examined through the regression model measured with respect to capital structure. The different financial ratios like Capital Structure Ratios (Total Debt to Equity Ratio and Long Term Debt to Equity Ratio) in addition to Profitability Ratios (Operating Profit Margin, Net Profit Margin, Return on Capital Employed, Return on Assets and Return on Equity) have been considered for the investigation. Both the capital structure as well as profitability ratios have shown significantly decreased over the span of ten years from 2005-06 to 2014-15. A significant declining trend in the long-term debt paying competence of ACC was observed during the period under study. Furthermore, all the measures of profitability ratios of the ACC stepped down remarkably by means of the passage of time during the study period. All these negative characteristics had definitely an adversarial impact on the overall long term solvency position of ACC. Correlation analysis revealed that both the capital structure ratios are highly correlated with all the profitability ratios. The regression analysis by taking total debt to equity ratio as dependent variable indicates that, there are statistically insignificant associations among total debt to equity ratioand the profitability ratios except ROA and ROE. On the other hand, the regression analysis by takinglong term debt to equity ratioas dependent variable reveals that, there are statistically insignificant associations among long term debt to equity ratioand the profitability ratios except ROE

REFERENCES

1. Aliakbar, R., Seyed, H. S. N., &Pejman, M. (2013). The relationship between capital structure decisions with firm performance: Comparison between big and small industries in firms listed at Tehran Stock Exchange.World of Sciences Journal, 1(9), 83–92.
2. Alom, K. (2013). Capital structure choice of Bangladeshi firms: An empirical investigation. Asian Journal of Finance & Accounting, 5(1), 320–333.
3. Chowdhury, A., & Chowdhury, S. P. (2010). Impact of capital structure on firm's value: Evidence from Bangladesh. Business and Economic Horizons, 3(3), 111–122. http://dx.doi.org/10.15208/beh.2010.32
4. Fama, E. F., & French, K. R. (2002). Testing trade-off and pecking order prediction, about dividends and debt.Review of Financial Studies, 15(1), 1–33. http://dx.doi.org/10.1093/rfs/15.1.1
5. Fosu, S. (2013). Capital structure, product market competition and firm performance: Evidence from South Africa. The Quarterly Review of Economics and Finance, 53(2), 140–151. http://dx.doi.org/10.1016/j.qref.2013.02.004
6. Gleason, K. C., Lynette, K M., & Ike, M. (2000). The Interrelationship between culture, capital structure, and performance: Evidence from European retailers. Journal of Business Research, 50(2), 185–191. http://dx.doi.org/10.1016/S0148-2963(99)00031-4
7. Margaritis, D., &Psillaki, M. (2010). Capital structure, equity ownership and firm performance. Journal of Banking & Finance, 34(3), 621–632. http://dx.doi.org/10.1016/j.jbankfin.2009.08.023
8. Mohamad, N. E. A. B., & Abdullah, F. N. B. A. (2012). Reviewing relationship between capital structure and firm's performance in Malaysia. International Journal of Advances in Management and Economics, 1(4), 151–156.
9. Saeedi, A., &Mahmoodi, I. (2011). Capital Structure and firm performance: Evidence from Iranian companies. International Research Journal of Finance and Economics, 70, 20–29.
10. Tianyu, H. (2013). The comparison of impact from capital structure to corporate performance between Chinese and European listed firms. Master's thesis of Jonkoping University. Retrieved from http://urn.kb.se/resolve?urn=urn:nbn:se:hj:diva-21994
11. Van Horne, J., &Wachowicz, J. (1995). Fundamentals of financial management (9th ed.). New Jersey: Prentice
12. Weston, J. F., & Brigham, E. F. (1979). Managerial finance. Holt, Rinehart and Winston.

Table-1 Capital Structure Ratios

Year	TDER	LTDER
2005-06	0.88	0.39
2006-07	0.69	0.19
2007-08	0.73	0.17
2008-09	0.68	0.15
2009-10	0.72	0.14
2010-11	0.65	0.14
2011-12	0.62	0.15
2012-13	0.55	0.13
2013-14	0.54	0.08
2014-15	0.52	0.07
Average	0.66	0.16
Maximum	0.88	0.39
Minimum	0.52	0.07

Table-2 Profitability Ratios

Year	OPM	NPM	ROCE	ROA	ROE
2005-06	26.03%	21.23%	34.49%	20.86%	39.19%
2006-07	24.85%	20.53%	35.15%	20.52%	34.64%
2007-08	24.39%	16.65%	30.92%	14.25%	24.61%
2008-09	29.63%	20.02%	34.31%	15.93%	26.71%
2009-10	19.67%	14.51%	20.64%	10.09%	17.31%
2010-11	17.35%	14.04%	19.92%	11.15%	18.43%
2011-12	13.79%	9.34%	18.16%	8.77%	14.37%
2012-13	11.45%	9.81%	14.76%	9.19%	14.00%
2013-14	10.34%	9.91%	13.70%	9.22%	14.19%
2014-15	7.22%	5.01%	9.43%	4.61%	7.01%
Average	18.47%	14.11%	23.15%	12.46%	21.05%
Maximum	29.63%	21.23%	35.15%	20.86%	39.19%
Minimum	7.22%	5.01%	9.43%	4.61%	7.01%

Table-3 Correlation Matrix

Particulars	TDER	LTDER	OPM	NPM	ROCE	ROA	ROE
TDNW	1.00						
LTDNW	0.89	1.00					
OPM	0.81	0.63	1.00				
NPM	0.84	0.72	0.96	1.00			
ROCE	0.81	0.70	0.97	0.97	1.00		
ROA	0.80	0.80	0.87	0.95	0.95	1.00	
ROE	0.85	0.85	0.87	0.95	0.94	0.99	1.00

Table-4 Regression Results for Total Debt to Equity Ratio as Dependent Variable and Various Factors as Predictors

Model Summary

Multiple R	R Square	Adjusted R Square	Standard Error
0.99	0.98	0.95	0.02

Goodness of Fit – ANOVA

Particulars	SS	MS	F	Significance F
Regression	0.10	0.02	38.45	0.00
Residual	0.00	0.00		
Total	0.11			

Regression Coefficients

Particulars	Coefficients	Standard Error	t Stat	P-value
Intercept	0.56	0.03	19.93	0.00
OPM	-3.23	2.40	-1.35	0.25
NPM	5.21	2.78	1.87	0.13
ROCE	2.34	1.72	1.36	0.24
ROA	-14.23	3.75	-3.80	0.02
ROE	5.67	0.83	6.81	0.00

Table-5 Regression Results for Long Term Debt to Equity Ratio as Dependent Variable and Various Factors as Predictors

Model Summary

Multiple R	R Square	Adjusted R Square	Standard Error
0.98	0.97	0.93	0.02

Goodness of Fit – ANOVA

Particulars	SS	MS	F	Significance F
Regression	0.07	0.01	25.16	0.00
Residual	0.00	0.00		
Total	0.07			

Regression Coefficients

Particulars	Coefficients	Standard Error	t Stat	P-value
Intercept	0.10	0.03	3.58	0.02
OPM	3.78	2.44	1.55	0.20
NPM	-4.59	2.82	-1.63	0.18
ROCE	-2.98	1.75	-1.70	0.16
ROA	-0.44	3.81	-0.12	0.91
ROE	3.57	0.85	4.23	0.01

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RESEARCH ARTICLE

Structural and Electronic Properties of ZnSe Using Density Functional Theory

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ABSTRACT

Semiconductor materials are the foundation of modern day's electronics for their properties like its reasonable speed, simple processing, useful temperature range etc. The modern science is also in the process of searching new varieties of semiconducting materials and upgrading the semiconductors which have already been made. Another interesting quality of semiconductors is that they can be doped with some impurities and their properties like conductivity can be controlled. Semiconductors are classified mostly according to their band gap and electrical conductivity. Semiconductor is technically neither an insulator nor a good conductor like metals. But it behaves like insulator at very low temperature and shows good conductivity at room temperature. At absolute zero temperature, the outermost energy band is completely filled, whether in case of conductor it is filled partially. Semiconductor have band gap, generally, less than 3 eV. Zinc selenide (ZnSe) is an attractive II-VI semiconducting material which has a large band gap of about 2.7-2.8 eV at room temperature (25°C). It earned good interest in recent years due to its wide applications in laser diodes, green-blue light emitting diodes. Zinc selenide (ZnSe) is also a valuable and perfect candidate for the application in solar cells, bio-medical tags. It is a promising material for lenses, output couplers, windows and optically controlled switching due to its low absorptivity at infrared wavelength, visible transmission. It can also be used for night vision applications. When cobalt is doped with ZnSe, the host material (ZnSe), in addition with semiconducting properties, develop magnetic properties in the same material. Collectively, ZnSe is a useful semiconductor and hence we use ZnSe in this work.

Keywords: Density functional theory, energy band, Zinc selenide

INTRODUCTION

Semiconductor materials are the foundation of modern day electronics for their properties like its reasonable speed, simple processing, useful temperature range etc. Modern science is always in the process of searching new varieties of semiconducting materials and upgrading the semiconductors which have already been made. Another interesting quality of semiconductors is that they can be doped with some impurities and their properties like conductivity can be controlled. Semiconductors are classified mostly according to their band gap and electrical conductivity. Semiconductor is technically neither an insulator nor a good conductor like metals. But it behaves like insulator at very low temperature and shows good conductivity at room temperature. At absolute zero temperature, the outermost energy band is completely filled, whether in case of conductor it is filled partially. Semiconductor have band gap, generally, less than 3 eV. In the contemporary science era, research work on another class of semiconductor is growing drastically because of their interesting and peculiar property. That is dilute magnetic semiconductor (DMS). They have some unique properties of having both magnetic and semiconducting properties in the same material. There are several naturally occurring magnetic elements like Chromium, Iron, Cobalt, Nickel. By introducing these into a semiconducting material as a dopant, they can introduce favourable magnetic properties in a controllable fashion. DMS are semiconductors doped with transition metal atoms or rare earth metal ions at very low concentration. After doping with suitable transition metal ions, the semiconducting material shows some peculiar properties. Zinc selenide (ZnSe) is an extrinsic semiconductor made by Zinc and selenium. It can behave as a dilute magnetic semiconductor when we dope a transition metal, like, we doped Cobalt in this work, and it show both magnetic and semiconducting nature. The present work focuses on structural and magnetic properties of Cobalt (Co) doped ZnSe. Zinc selenide (ZnSe) is an attractive II-VI semiconducting material which has a large band gap of about 2.7-2.8 eV at room temperature (25°C). It earned good interest in recent years due to its wide applications in laser diodes, green-blue light emitting diodes. Zinc selenide (ZnSe) is also a valuable and perfect candidate for the application in solar cells, bio-medical tags. It is a promising material for lenses, output couplers, windows and optically controlled switching due to its low absorptivity at infrared wavelength, visible transmission[1,2,3,4]. It can also be used for night vision applications. When cobalt is doped with ZnSe, the host material (ZnSe), in addition with semiconducting properties, develop magnetic properties in the same material. Collectively, ZnSe is a useful semiconductor and hence ZnSeis chosen in this work.

COMPUTATIONAL METHOD

Here the calculations are based on the DFT in the LDA. Only valence electrons are explicitly considered. Their interaction with the atomic cores is treated by ab initio Vanderbilt pseudo-potentials [5]. The code chosen here is the Quantum Espresso code. It's a first principle total energy code that uses both norm-conserving and Vanderbilt pseudo-potential. The softest possible pseudo-potential is constructed and used. The pseudo-potential scheme used allows the expansion of the single particle wave functions into a plane wave basis set. It is restricted by a kinetic energy cut off of 28.0 Ry. This restriction corresponds to about 160 plane waves per atom. A set of special 2×2×2, 4×4×4,8×8×8 and 10×10×10 k-points generated by the Monkhorst-Pack scheme is used for BZ sampling.

The exchange and correlation energy per electron is described by Monte Carlo results of Ceperley and Alder [6] in the parametrization of Perdew and Zunger[7]. In order to avoid errors due to the use of frozen cores nonlinear core correction to the exchange-correlation energy [8] are included in the generation of pseudo-potentials. The single particle Kohn-Sham [8] equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels. Quantum espresso [9] is an open source package under the terms of General Public License for the electronic structure calculations. Density functional theory andits approximations are all implemented in this program which enables calculation of quantum mechanical systems. Hence, it is very practical for crystal structure and surface structure calculations which are the main tool of quantum chemistry measurements. Quantum espresso package is written mostly in Fortran 95, C and Fortran 77. Parallel computation is done which reduces computational

cost considerably.Theseuseful implementations are ground state energy calculation of Kohn Sham orbitals,pseudo-potential approximations for the exchange correlation potentials, supercell approach, structural optimization schemes, ab initio molecular dynamics schemes, calculation of magnetic systems, density functional perturbation theory calculations etc. It has several different codes in it which are devoted for different type of calculations like self-consistent field calculations, phonon calculations etc.

RESULTS AND DISCUSSION

Density functional theory (DFT) [10, 11,12] calculation was done for electronic properties of ZnSe. ZnSe crystallizes in zinc blend structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei. To begin with, primitive unit cells with 2 atoms is considered the to make the computational calculation easier to handle. The total energy calculation, band structure calculation was done and band structure, charge density distribution and the density of states of ZnSe was plotted.

Structural Properties

The first principle pseudo-potential calculations were done by using QE code for structural and electronic properties of ZnSe. ZnSe is a face-cantered cubic crystal, and a primitive unit cell is used in all the calculations. It contains two atoms, a Zn atom at its origin and a Se atom located in the main diagonal of cubic unit cell, at a distance equal to one fourth of its size. The crystal structure and corresponding BZ are shown in the figure below, with some special k-points indicated. The calculation was started to find out the lattice constant `a` for cubic ZnSe by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. To start with, different values of possible lattice constants were taken, performed the self-consistencefield (SCF) calculation to find out the corresponding energy. Then the volume versus total energy graph was plotted which is shown in Fig. (1). The minimum energy value in the graph corresponds to the volume 311 $Bohr^3$. Thus, the calculated lattice constant for ZnSe is 10.74 Bohr. The experimental lattice constant value for cubic ZnSe is 10.71 Bohr. So our calculated value is in good agreement with the experimental value.The charge density plot shows the distribution of fractional charges from which information about the strength of bonding, piling and depletion of charges can be known. Fig. (2) shows the 2-dimensional charge density plot of cubic ZnSe in contour lines plus grey levels from LDA calculations. The electronic charge density of different regions is indicated in the shaded baron the right hand side of the figure. Electronic density is constant along any curve in the Fig. (2). ZnSe is covalently bonded. The charge density is strongly accumulated around Se atom which is a result of strong2p potential of Se. Some charges around the Zn atom move to the bonding region which gives rise to the ionic character of ZnSe. The charge transfer into the bonding region causes a decrease in the total energy. The bonds between Zn and Se are stable which causes the stabilization of zincblende structure. The charge density plot obtained by can be compared with the plot reported by Van de Walleis shown in figure. Comparing these two can be seen that our calculated results are in good comparison with the reference results. The total energy calculated to be = -17.32409323 Ry. As explained above, the total energy consists of the energy contribution from each electron, the exchange and correlation energy, the Hartree contribution and the Ewald contribution. The values obtained in our calculation are as follows

Total energy = -17.32409323 Ry
One-electron contribution= 2.72819257
Hartree contribution= 1.55869453
Exchange and Correlation contribution= -4.76660671
Ewald contribution= -16.84437362

Electronics Structure

The calculated energy band structure of cubic ZnSe along directions of high symmetry is shown in Fig. (3). we have calculated the band energy for the valence and conduction band using DFT within LDA. The electronic configuration

of Zn is [Ar]3d10 4s2 and electronic configuration of Se is [Ar]3d10 4s2 4p4. For this calculation, 4s2 electrons of Zn and 4s2 4p4 electrons of Se are considered as the valence electron. Pseudo-potential for Zn and Se are used to obtain a smooth potential value. This helped in reducing the calculation effort. This calculations correctly predict that the valence band maximum and conduction band minimum occurs at Gamma point of the BZ, indicating a direct band gap. This is in accordance with experimental results shown in figure (3). Both valence band and conduction band positions are in good agreement with the reference results. The calculated band gap is 1.6 eV. The band gap of cubic ZnSe is 2.54 eV which can be seen from figure (3). The smallerband gap compared to experimental value is due to the inherent drawbacks of LDA.

The band gap value reported by Laihia using X-ray diffraction data is 2.0 eV. This shows our result is having an error of 20% in comparison to experimental X-ray diffraction data. However, the overall band profiles are in good agreement with other results. Comparison of the present work with other experimental and theoretical result was depicted in Table I. The total density of states (DOS) of un doped ZnSe from LDA calculations using pseudo-potential are shown in fig (5.7). The left side represents the valence band (VB) which ends at 0 eV on the fig. Actually, the top of valence band is taken as 0 eV for reference purpose and the diagram is plotted. The major part of Se-s and p and a small part of Zn-s and states contributes towards the VB. A combination of Zn-s and Se-sp stated form the lower portion of the conduction band (CB). The total energy, the Fermi energy, the position of bands, etc., all are found to be same in both cases. The DOS plot also shows that there is no difference in the peaks and the energy gap due to relaxation which means relaxation does not cause the atoms to move away from their position and this exactly is what expected.

CONCLUSIONS

The first principle DFT calculations were done to study the structural and electronic properties of cubic ZnSe. The values of different parameters like, lattice constant, band gap, band plot, charge distribution and density of states were calculated and summarized the observations as follows. The description of interacting many-particle systems is, in general, very complicated and approximations need to be made. Several methods in quantum physics try to describe the motion of the electrons in such systems by the electronic wave function, the solution of either the time-independent or time-dependent Schr¨odinger equation. The computational effort involved in these methods, is very high. In contrast to density-functional theory, the computational costs are much lower. In DFT, the electronic wave function is not evaluated for a full description of the interacting many-particle system but it is sufficient to look at the electron density. The implementation of such a perturbation theory scheme was discussed in depth in chapter 3; it was shown that it is relatively easy to implement such a scheme within the plane wave pseudo-potential framework when working within a structured code such as Quantum Espresso. The structure of the DFPT code is such that it is relatively easy to extend; for example, various XC functionals, aside from LDA and GGA could be implemented with only a little effort. Using DFT the calculated results with the help of Quantum Espresso it is found that these results are in good agreement with other theoretical and experimental results. The lattice constant of ZnSe is calculated with energy minimization method. This value is used for further calculations. The charge density distribution was checked to know the bonding between the elements forming the compound. The band structure calculation and plotting of the band structure was done. The band gap was found out. This study revealed that ZnSe is an indirect band gap semiconductor. The Fermi energy for ZnSe and plotted the density of states were established. The results obtained here can be used as a basis for further investigation of properties of ZnSe.

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REFERENCES

1. P Mallikarjuna, J Sivasankar, M RiganaBegam, N Madhusudhana Rao, S Kaleemulla, et al.. Structural, Optical and Magnetic Properties of Co doped ZnSePowders . Mechanics, Materials Science Engineering Journal, Magnolithe, 2017.
2. B. Amin, S. Arif, I. Ahmad, M. Maqbool, R. Ahmad, S. Goumri-Said, K. Prisbrey, Cr-Doped III–V nitrides: potential candidates for spintronics, Journal of Electronic Materials, 40 (2011) 1428-1436, DOI: 10.1007/s11664-011-1539-7.
3. H. Ohno, Making Nonmagnetic Semiconductors Ferromagnetic, Science, 281 (1998) 951, DOI: 10.1126/science.281.5379.951.
4. S.A. Wolf, D.D. Awschalom, R.A. Buhrman, J.M. Daughton, S. von Molnár, M.L. Roukes, A.Y. Chtchelkanova, D.M. Treger, Spintronics: A Spin-Based Electronics Vision for the Future, Science, 294 (2001) 1488, DOI: 10.1126/science.1065389.
5. D. Vanderbilt, Phy. Rev. B 41, 7892(1990).
6. D. M. Ceperley and B. I. Alder, Ground State of the Electron Gas by a Stochastic Method, Phys. Rev. Lett. 45,566(1980)
7. J.P. Perdew and A. Zunger, Self-interaction correction to density-functional approximations for many-electron systems, Phys. Rev. B 23, 5048 (1981).
8. W.Kohn and I.J .Sham,Phys.Rev.140,(1965)
9. P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. BuongiornoNardelli, M.Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carn-imeo, A. Dal Corso, S. de Gironcoli, P. Delugas, R. A. DiStasio Jr, A. Ferretti, A.Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, JJia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. K¨u¸c¨ukbenli, M .Lazzeri, M. Marsili, N.Marzari, F. Mauri, N. L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto,S. Ponc´e, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, S. Baroni J.Phys.:Condens.Matter 29, 465901 (2017)
10. K.J Chang and M.L.Cohen,P hys.Rev.Lett.35,8196(1987)
11. P. Villars and L. D. Calvert, (ASM International, Cleveland, 1991).
12. D. Vanderbilt, Phy. Rev. B 41, 7892(1990).

Table: I comparison of the work with other experimental and theoretical result

Parameter	Our calculation	Reference (Expt/Theoretical)
Lattice constant	10.74 Bohr	10.71 Bohr
Band gap	1.6 eV	2.0 eV
Total energy	-17.32409323 Ry	
Fermi energy	4.5847 eV	
Charge density plot	Fig 2	In good agreement
Density of states	Fig 3	In good agreement

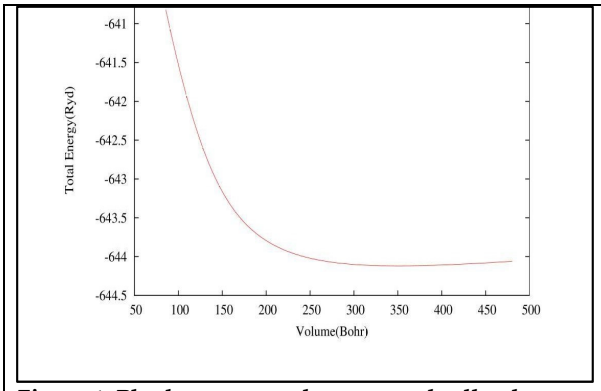

Figure 1: Plot between total energy and cell volume to determine lattice constant for ZnSe

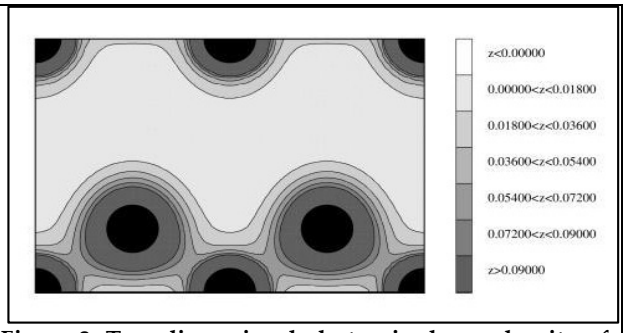

Figure 2: Two dimensional electronic charge density of ZnSe. Electronic density of different shaded regions is indicated on the bar. This is the result of LDA calculations.

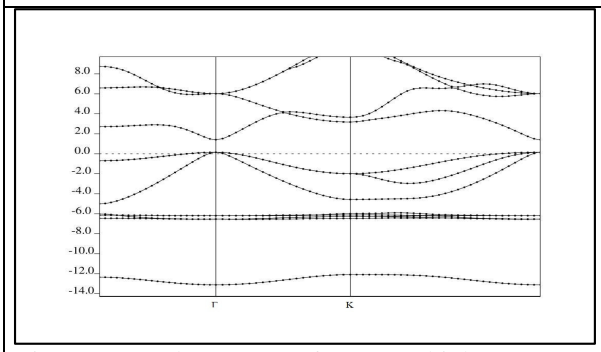

Figure 3: Band structure of ZnSe at high symmetry points from PBE calculations. Top of the valence band wastaken as zero on the energy axis. The dashed line showed the top of the valence band

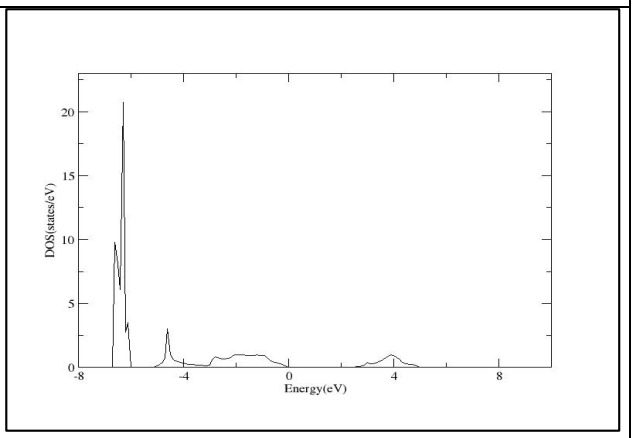

Fig 4: The total density of states of ZnSe

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RESEARCH ARTICLE

Density Functional Theory Calculations of Electronic Properties of InP

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ABSTRACT

This work has been done by using Density functional theory (DFT) method to study the structural and electronics properties of Indium phosphide (InP). Owing to its wide band gap and few other properties, Indium phosphide is a suitable candidate for the application in solar cells, optical fibre, bio-medical tags, robotics and scanning system. It is a promising material for lenses, output couplers, windows and optically controlled switching due to its low absorptivity at infrared wavelength, visible transmission. Collectively, InP is a useful semiconductor and hence we use InP in this work. Using the first principle DFT, different parameters like lattice constant, band gap, band plot, charge distribution and density of states were calculated. The band structure calculations were done and plotted too. The band gap was found out. InP has a direct band gap.

Keywords: Density functional theory, energy band, Indium Phosphide

INTRODUCTION

Now a day's Condensed Matter Physics is one of the largest research field in Physics. The fast growing technological progress is closely related to the development of various materials and tools made from those materials. Semiconductor materials are the foundation of modern day's electronics for their properties like its reasonable speed, simple processing, useful temperature range etc. The material science research is always in the process of searching new types semiconducting materials and upgrading the semiconductors which are already in use. Another interesting quality of semiconductors is that they can be doped with some impurities and their properties like conductivity can be controlled. Semiconductors are classified mostly according to their band gap and electrical conductivity. Semiconductor is technically neither an insulator nor a good conductor like metals. But it behaves like

insulator at very low temperature and shows good conductivity at room temperature. In today's there are group of III-V family of compound semiconductor provides the material basis for the development of electronic and optoelectronic device. Recently there has been much interest in the field InP. It is binary III-V semiconductor compound which made both indium and phosphorus is very popular in optoelectronics field and microelectronic field. Knowledge of the InP is important because of its increasing application in various optoelectronic field. It is used in the manufacturing of device such as diodes (LED, laser light, electroluminescent), transistor (WT, FET and field effect) and optical amplifier. The realization of InP hetero junction bipolar transistor is an important issue in the development of optical fiber communication system (20-40Gbit/s) [1]. Optical characteristics are required for the optimal device operation-ray photo emission spectroscopy was used in the InP studied by Ley et al. [2]. Aspens and Stuand [3] measured the dielectric function of InP with other III-V semiconductor compound separated by ellipsometry between 1.5 and 6.0eV. In this paper, we report theoretical study of the structural and electronics properties of InP. Several studies have been conducted using the MBJ potential to calculate the structural and electronic properties of different solid. Our calculation is based on the DFT method and solves all the calculation using Quantum Espresso code. These calculations of electronic band structure and properties were performed using Local-density-approximation (LDA) [4] and generalized gradient approximation [GGA][5].

Computational Method

Here the calculations are based on the DFT in the LDA. Only valence electrons are explicitly considered. Their interaction with the atomic cores is treated by ab-initio Vanderbilt pseudopotential [8]. The code chosen here is the Quantum Espresso code. It's a first principle total energy code that uses both norm-conserving and Vanderbilt pseudopotential. The softest possible pseudopotential is constructed and used. The pseudopotential scheme used allows the expansion of the single particle wave functions into a plane wave basis set. It is restricted by a kinetic energy cut off of 28.0 Ry. This restriction corresponds to about 160 plane waves per atom. A set of special 2×2×2, 4×4×4, 8×8×8 and 10×10×10 k-points generated by the Monkhorst-Pack[9] scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Monte Carlo results of Ceperley and Alder [10] in the parameterization of Perdew and Zunger. In order to avoid errors due to the use of frozen cores nonlinear core correction to the exchange-correlation energy[11] are included in the generation of pseudopotential. The single particle Kohn-Sham [12] equations are solved and the eigenvalues are taken to interpret bulk band structure and the vacancy levels. Quantum Espresso [13] is an open source package under the terms of General Public License for the electronic structure calculations. Density functional theory and its approximations are all implemented in this program which enables calculation of quantum mechanical systems. Hence, it is very practical for crystal structure and surface structure calculations which are the main tool of quantum chemistry measurements. Quantum espresso package is written mostly in FORTRAN 95 and C and Fortran 77. Parallel computation is done which reduces computational cost considerably. These useful implementations are ground state energy calculation of KohnSham orbitals, pseudopotential approximations for the exchange correlation potentials, super cell approach, structural optimization schemes, ab initio molecular dynamics schemes, calculation of magnetic systems, density functional perturbation theory calculations etc. It has several different codes in it which are devoted for different type of calculations like self-consistent field calculations, phonon calculations.

RESULTS AND DISCUSSION

The DFT method is used to study of the structural and electronic properties of the binary compound InP. The method of pseudopotential based density functional theory (DFT) was used. The calculations were done by the code Quantum espresso. This calculation of the electronic band, structure and density of states (DOS) were performed using local-density approximation (LDA). InP is likely to crystallize as a function of applied pressure. Indeed, materials crystallize in different phases and have the ability to transform from one phase to another under the effect of temperature or pressure. The calculation of the total energy allows us to have the static equilibrium properties. InP

crystallizes in the zinc-blende structure. The primitive unit cell of two atoms with zinc-blende structure was chosen for this work. The calculations are carried by forming a cube of a side 'a', where 'a' is the lattice constant of the Bravais lattice. These calculations require the determination of wave functions and positions of 8 electrons and 2 nuclei. The ZB phase was chosen since it has fewer atoms per unit cell, and is therefore computationally easier to handle. In the band structure calculations, the valence electronic configurations assumed for the atoms of InP are: In 5p1 and P 3p3. The semi core 4d electrons of In were found to have as valence electrons and essential to describe accurately structural properties. The ground state properties are found asfollows.
Indium phosphide is face-centered cubic crystal structure has composed of two sub lattice. Its appearance like black cubic crystal structure and it is also Zinc-blended cubic crystal structure.

Structural Properties

The first principle pseudopotential calculations using QE code were done for structural and electronic properties of InP. For cubic polytypic of InP, a face-centered cubic crystal, and a primitive unit cell is used in all the calculations. It contains two atoms, an Indium atom at its origin and a Phosphorus atom located in the main diagonal of cubic unit cell, at a distance equal to one fourth of its size. The crystal structure and corresponding BZ are shown in Fig. 1. The calculation of lattice constant 'a' for cubic InP was done by energy minimization method. The lattice constant value obtained in the present calculation found to be in good agreement with the experimental value which is8.77950A. The minimization of curves that represent the variation of the total energy as a function of the volume V of the unit cell, for phases studied using LDA approximations for InP is shown. The minimum energy value in the graph corresponds to the volume 245 $Bohr3$. Thus, the calculated lattice constant for InP is 5.8687 Bohr. The experimental lattice constant value for cubic InP is 5.8687 Bohr. So our calculated value is in good agreement with the experimental value. The charge density plot shows the distribution of fractional charges from which information about the strength of bonding, piling and depletion of charges can be known. Fig. 3 shows the 2- dimensional charge density plot of cubic InP in contour lines plus grey levels from LDA calculations. The electronic charge density of different regions is indicated in the shaded baron the right hand side of the figure. Electronic density is constant along any curve in the Fig. 3. InP is covalently bonded. The charge density is strongly accumulated around p atom which is a result of strong 5p potential of In. Some charges around the In atom move to the bonding region which gives rise to the ionic character of InP. The charge transfer into the bonding region causes a decrease in the total energy. The bonds between In and P are stable which causes the stabilization of zinc blende structure. The total energy calculated to be = -415.925 Ry. As we know, the total energy consists of the energy contribution from each electron, the exchange and correlation energy, the Hartree contribution and the Ewald contribution. The values obtained in our calculation are as follows.
Total energy = -415.925 Ry
One-electron contribution= -51.248769Ry
Hartree contribution= 34.69500434
Exchange contribution= -50.04418018
Ewald contribution= -89.60297548

Electronics Structure

The calculated energy band structure of cubic InP along directions of high symmetry is shown in Fig. 4. The band energy for the valence and conduction band were calculated using DFT within LDA. The electronic configuration of In is Kr $4d^{10}5s^{2}5p^{1}$and electronic configuration of P $1s^{2}2s^{2}2p^{6}3s^{2}3p^{3}$. The electron in the levels $5p^{1}$of In and $3p^{3}$of P were considered as the valence electron for our calculation. Pseudopotential has been for In and P to obtain a smooth potential value. This helped in reducing the calculation effort. The band plot obtained is shown in Fig. 4. This calculations correctly predicts that the valence band maximum and conduction band minimum occurs at Gamma point of the BZ, indicating a direct band gap. This is in accordance with experimental results too. Both valence band

and conduction band positions are in good agreement with the reference results [22]. The calculated band gap is 1.26 eV. The experimental band gap reported for cubic InP is 1.48 eV. The smaller band gap compared to experimental value is due to the inherent drawbacks ofLDA. This shows our result is having an error of 14% comparison to experimental data is good experiment. However, the overall band profiles are in good agreement with other results. The total density of states (DOS) of InP from LDA calculations using pseudopotential are shown in fig 5.7. The left side represents the valence band (VB) which ends at 0 eV on the fig. Actually the top of valence band is taken as 0 eV for reference purpose and the diagram is plotted. The major part of P-s and p and a small part of In-s and states contributes towards the VB. A combination of In-s and P-sp states, form the lower portion of the conduction band (CB). The total energy, the Fermi energy, the position of bands, etc., all are found to be same in both cases. The DOS plot also shows that there is no difference in the peaks and the energy gap due to relaxation which means relaxation does not cause the atoms to move away from their position and this exactly is what expected.

CONCLUSIONS

The first principle DFT calculations are done to study the structural and electronic properties of cubic InP. Different parameters like, lattice constant, band gap, band plot, charge distribution and density of states were calculated. The work done can be summarized as follows. The description of interacting many-particle systems is, in general very complicated and approximations need to be made several methods in quantum physics try to describe the motion of electrons in such systems by the electronic wave function, the solution of either the time independent or time – dependent Schrodinger equation. The computational effort involved in these methods is very reasonable. Using DFT the calculated results with the help of Quantum Espresso we have found results in good agreement with other theoretical and experimental results. The lattice constant of InP is calculated with energy minimization method. This value is used for further calculations. We checked the charge density distribution to know the bonding between the elements forming the compound. We did the band structure calculation and plotted the band structure too. The band gap was found out. It also gave us information that InP is a direct band gap semiconductor. We found out the Fermi energy for InP and plotted the density of states. The results obtained here can be used as a basis for further investigation of properties of InP.

ACKNOWLEDGMENT

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REFERENCES

1. M. J. W. Rodwell, M. Urteaga, Y. Betser, T. Methew, P. Krishnan,D. Scott, S. Jaganathan, D. Mensa, J. Guthrie, P. Pullela, Q. Lee, B.Agarwal, U. Bhattacharya, S. Long, S. C. Martin, and R. P. Smith,"Scaling of InGaAs/INALAL HBTs for high speed mixed-signal andmm-wave ICs,"Int. J. High Speed Electron. Syst., vol. 11, pp. 159–215,2001
2. L. Ley, R.A. Pollak, F.R. Mcfeely, S.P. Kowalazyk, D.A. Shirely, Total valence-band densities of states of III-V and II-VI compounds from x-ray photoemission spectroscopy, Phys. Rev. B 9 (1974) 600.
3. D.E. Aspnes, A.A. Studna, Dielectric functions and optical parameters of Si, Ge, GaP, GaAs, GaSb, InP, InAs, and InSb from 1.5 to 6.0 eV, Phys. Rev. B27 (1983) 985
4. J.P. Perdew, Y. Wang, Phys. Rev. B 45 (1992) 13244.
5. J.P. Perdew, K. Burke, M. Emzerhof, Phys. Rev. Lett. 77 (1996) 3865
6. Michela R. squillante, Kanais. shan, in semiconductor and semimetals, 1995
7. Michela R.squillante, Kanais. shan, in semiconductor and semimetals, 1995
8. Shmidt Handbook Series on Semiconductor Parameters, vol.1, M. Levinshtein,

9. S. Rumyantsev and M. Shur, ed., Handbook Series on Semiconductor Parameters , World Scientific, London, 1996, pp. 169-190.
10. Dargys A. and J. Kundrotas Handbook on Physical Properties of Ge, Si, GaAs and InP, Vilnius, Science and Encyclopedia Publishers, 1994
11. Sheng Chao, Tien; Lee, Chung Len; Lei, Tan Fu (1993), Journal of Materials Science Letters,12 (10):721, doi:10.1007/BF00626698
12. Indium Phosphide and Indium Gallium Arsenide Help Break 600 Gigahertz Speed Barrier. April 2005.
13. The Light Brigade appeared in Red Herring in 2002. Archived June 7, 2011, at the Wayback Machine.
14. D. Vanderbit, Phys.Rev.B41,7892(1900)
15. H. J. Monkhorst and J. D. PACK,PHYS. Rev. B 13,5188(1976)
16. D. M. Ceperley and B. I. Alder, Phys.Rev.Lett.45,566(1980)
17. S. G. Louie, S. Froyen and M.L Cohen, Physc.Rev. B 26,1738(1982)
18. W. Kohn and I. J. Sham,physc.Rev.140,(1965)
19. P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. BuongiornoNardelli, M.Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carn-imeo, A. Dal Corso, S. de Gironcoli, P. Delugas, R. A. DiStasio Jr, A. Ferretti, A.Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, JJia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. K¨u¸c¨ukbenli, M .Lazzeri, M. Marsili, N.Marzari, F. Mauri, N. L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto,S. Ponc´e, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, S. Baroni J.Phys.:Condens.Matter 29, 465901 (2017)

Table : II comparison of the work with other experimental and theoretical result

Parameter	Our calculation	Reference (Expt/Theoretical)
Lattice constant	5.86Bohr	11.09*B*ohr
Band gap	1.26eV	1.48ev
Total energy	-415.925	NA
Fermi energy	6.7959	NA

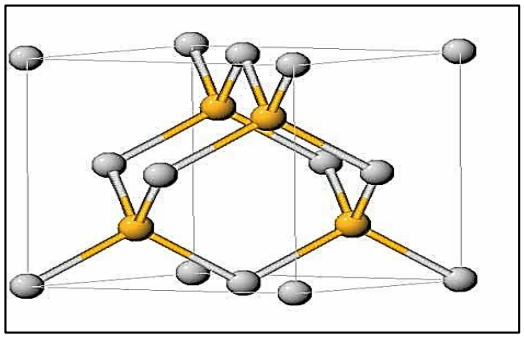

Fig 1: zinc blended structure of InP (In as graycolor and P as yellow color)

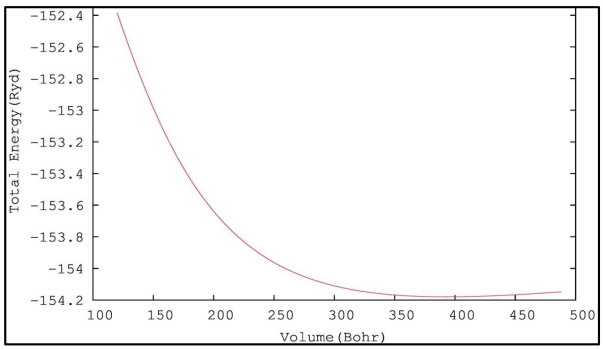

Fig 2: Plot between total energy and cell volume to determine lattice constant for InP

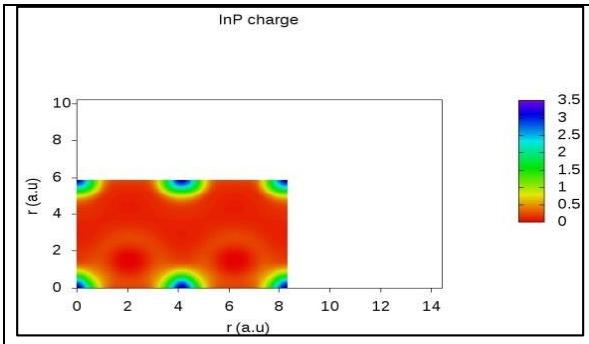

Fig 3: Two dimensional electronic charge density of InP Electronic density of different shaded regions are in on the bar. This is the result of LDA calculation.

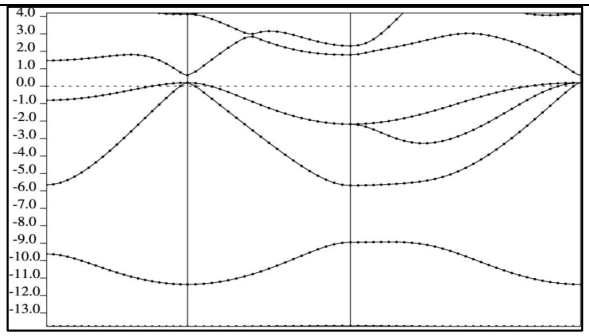

Fig 4: Band structure of InP at high symmetry points from PBE calculations. Top of the valence band is taken as zero on the energy axis. The dashed line shows the top of the valence band.

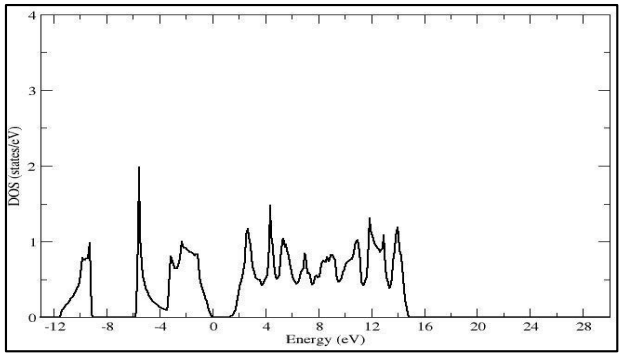

Fig 5: The total density of states of InP from as calculation using LDA. Top of the valence band is taken as zero.

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RESEARCH ARTICLE

First Principle Calculations of Structural and Electronic Properties of ZnO

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ABSTRACT

Calculations from first principles Density functional theory (DFT) has been used to study the structural and electronics properties of Zinc Oxide (ZnO). Semiconductor materials are the foundation of modern days electronics for their properties like its reasonable speed, simple processing, useful temperature range etc. Another interesting quality of semiconductors is that they can be doped with some impurities and their properties like conductivity can be controlled. ZnO is also a valuable and perfect candidate for the application in solar cells, bio-medical tags, robotics, and scanning system. It is a promising material for lenses, output couplers, windows and optically controlled switching due to its low absorptivity at infrared wavelength, visible transmission. Collectively, ZnO is a useful semiconductor and hence ZnO is used in this work. Using the first principle DFT, different parameters like lattice constant, band gap, band plot, charge distribution and density of states were calculated. The band structure calculation were done and plotted too. The band gap was found out. ZnO has a direct bandgap.

Keywords: Band gap, density functional theory, semiconductor materials, ZnO

INTRODUCTION

Condensed matter physics is an important input for science and technology. Now a days it is one of the largest research fields in physics. This field studies material properties from the nano-scale to the macroscopic level experimentally and theoretically. Before zinc was recognized as a unique element, it was used to make brass by the Romans in the first century A.D. It was not until the 14th century that zinc was recognized as a metal in Zewar. ZnO was created as a by-product of the smelting process [1]. The white powder proved to be useful as a remedy for sore

eyes. The zinc smelting technique was taken talk to China in the 16th or 17th century where it was used to produce brasses with high zinc contents. Europeans imported zinc from China shortly after words and it was listed as an element on the periodic table by Antoine Lavoisier in 1789[2]. Before electrical and optical properties were utilized. The color of zinc oxide is always white. Perhaps the first use of ZnO for electronic applications was in build in 21 centuries. Semiconductors are classified mostly according to their band gap and electrical conductivity. Semiconductor is technically neither an insulator nor a good conductor like metals. But it behaves like insulator at very low temperature and shows good conductivity at room temperature. At absolute zero temperature (0K), the outermost energy band is completely filled, whether in case of conductor it is filled partially. Semiconductor have band gap, generally, less than 2.1eV. ZnO is an attractive II-IV semiconducting material which has a large band gap of about 3.37 eV at room temperature. It earned good interest in recent years due to its wide applications in laser diodes, green-blue light emitting diodes.

Zinc oxide is a II and IV group semiconductor and it is a wide band gap (2.27eV) semiconductor, which absorbs UV light [3]. Zinc oxide (ZnO) is generally n-type semiconductors, which has a direct wide band gap (3.37 eV at room temperature) and free exciton binding energy of 60 meV in comparison with the room thermal energy of 26 meV [4]. During the last several decades, wide band gap receives great interest from the scientific due to their potential application. Zinc oxide materials are widely studied by researchers due to their many important technological applications such as optoelectronics, magneto-electronics, highly efficient blue LEDs and microwave devices [5, 6]. As a multifunctional material, the wide range of their properties displayed by ZnO has been recognized for a longer. With its strong luminescence, ZnO can be used in light emitting devices, laser diode and phosphor [7, 8], such as light-emitting diode , ZnO offers unique photo catalytic properties, making it possible for this oxide to be used as a photo catalyst in the process of degradation of various pollutants [9]. In recent years, much attention has been given to theoretical studies on metal oxide clusters. Experimental studies of metal oxides have been matched by theoretical calculations. Density functional theory (DFT) and other theoretical methods provided geometry optimization [10] of ZnO and allowed to study band gaps [11] and spectroscopy properties (UV – Vis, IR, Raman and NMR) of metal oxides. Electrical and optical properties of hydrothermally grown ZnO crystal, as well as structural changes at its surface have been investigated before and after irradiation by pulsed Nd:YAG laser. The origin of experimentally observes the n-type semi conductivity origin from Zn interstitials was explained. Controlled formation of Zn and ZnO nanoparticles by laser radiation was calculated.

Computational Method

Here the calculations are based on the DFT in the Local Density Approximation (LDA). Only valence electrons are explicitly considered. Their interaction with the atomic cores is treated by ab initio Vanderbilt pseudopotentials [12]. The code chosen here is the Quantum Espresso [13] code. Density functional theory and its approximations are all implemented in this program which enables calculation of quantum mechanical systems. It's a first principle total energy code that uses both norm-conserving and Vanderbilt pseudopotential. The softest possible pseudopotential is constructed and used. The pseudopotential scheme used allows the expansion of the single particle wave functions into a plane wave basis set. It is restricted by a kinetic energy cut off of 28.0 Ry. This restriction corresponds to about 160 plane waves per atom. A set of special 2×2×2, 4×4×4, 8×8×8 and 10×10×10 k-points generated by the Monkhorst-Pack [14] scheme is used for BZ sampling. The exchange and correlation energy per electron is described by Monte Carlo results of Ceperley and Alder [15] in the parameterization of Perdew and Zunger [16]. In order to avoid errors due to the use of frozen cores nonlinear core correction to the exchange-correlation energy [17] are included in the generation of pseudopotentials. The single particle Kohn-Sham [18] equations are solved and the Eigen values are taken to interpret bulk band structure and the vacancy levels.

RESULTS AND DISCUSSION

Density functional theory (DFT) calculation was done for electronic properties of ZnO. ZnO crystallizes in cubic zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant

of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei. To begin with, we have considered the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The band structure was designed, calculated and plotted along withthe plotted charge density distribution and the density of states of ZnO

Structural Properties

The first principle pseudo-potential calculations using QE code for structural and electronic properties of ZnO is done. It is a face-centered cubic crystal, and a primitive unit cell is used in all the calculations. It contains two atoms, a Zn atom at its origin and a O atom located in the main diagonal of cubic unit cell, at a distance equal to one fourth of its size. The crystal structure and corresponding BZ are shown in the figure below, with some special k-points indicated. The ZnO crystal structure is compound of two sub lattice. The structure of Zinc oxide has the Wurtzite Hexagonal Crystal structure.Zinc oxide shows the crystal structure under electron microscopes when examined further. The exact shape of the crystal depends on the method of formation. The calculation was started to find out the lattice constant `a` for cubic ZnO by energy minimization method. The lattice constant value obtained in the present calculation is in good agreement with the experimental value which is 6.3306$\AA^0$.

The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. This work started with different values of possible lattice constants, performed the self consistence field (SCF) calculations to find out the corresponding energy. The energy minimization method is used here to find the lattice constant. Thus, the calculated lattice constant for ZnO is 6.30 Bohr. The experimental lattice constant value for cubic ZnO is a=3.2495$\AA^0$ c=5.2069$\AA^0$. So our calculated value is in good agreement with the experimental value. The charge density plot shows the distribution of fractional charges from which information about the strength of bonding, piling and depletion of charges can be known. Fig. (3) shows the 2-dimensional charge density plot of cubic ZnO in contour lines plus grey levels from LDA calculations. The electronic charge density of different regions is indicated in the shaded baron the right hand side of the figure. Electronic density is constant along any curve in the Fig. (3). ZnO is covalently bonded .The charge density is strongly accumulated around Zn atom which is a result of strong 4s potential of Zn and 2p potential of oxygen. Some charges around the Zn atom move to the bonding region which gives rise to the ionic character of ZnO. The charge transfer into the bonding region causes a decrease in the total energy. The bonds between Zn and O are stable which causes the stabilization of zinc blend structure. The charge density plot obtained by us is in good comparison with the reference results.

The total energy calculated to be = -317.46309515 Ry. As we know, the total energy consists of the energy contribution from each electron, the exchange and correlation energy, the Hartree contribution and the Ewald contribution. The values obtained in our calculation are as follows:
Total energy = -317.46309515 Ry
One-electron contribution= -175.97820289 Ry
Hartree contribution= 122.81435422 Ry
Exchange and Correlation contribution= -51.19568039 Ry
Ewald contribution= -213.10356609 Ry

RESULTS ON ELECTRONICS PROPERTIES

The electronic structure calculations are done by using Quantum Espresso with DFT. The lattice constant mentioned above is used here for all calculations. Different k point samplings are used for calculations. The Fermi energy (EF), band gap, type of band gap, total and partial DOS, and the width of the valence and conduction bands are important information that can be extracted from electronic and structure calculations. It is very important to use a large number of k points to calculate the electronic band structure as the details of the electronic band structure come from

integrals ink-space. The calculated energy band structure of cubic ZnO along directions of high symmetry is shown in Fig. 3. All calculated band energy for the valence and conduction band are done using DFT within LDA. The electronic configuration of Zn is [Ar] 3d10 4s2 and electronic configuration of O is [He] 2s2 2p4. We have considered 4s2 electrons of Zn and 4s2 4p4 electrons of O as the valence electron for our calculation. We have used pseudopotential for Zn and O to obtain a smooth potential value. This helped in reducing the calculation effort. we present the calculated electronic band structure of zinc-blende ZnO at the predicted equilibrium lattice constant along the selected high symmetry k path within the first Brilloiun zone of its primitive cell, and in Table 1, we list the energy difference between the bottom of the conduction and the top of the valence band at high symmetry points in the Brillouin zone as determined from the periodic BAND program. Our calculations correctly predicts that the valence band maximum and conduction band minimum occurs at Gamma point of the BZ, indicating a direct band gap. This is in accordance with experimental results. Both valence band and conduction band positions are in good agreement with the reference results. The calculated band gap is 2.1eV. The band gap of cubic ZnO is 3.3 eV which can be seen from Fig. 6. The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA. At the point Γ the highest valence band is doubly degenerate. The band gap value reported by Laihia using X-ray diffraction data is 2.0 eV. This shows our result is having an error of 20% in comparison to experimental X-ray diffraction data. However, the overall band profiles are in good agreement with other results. The underestimation of the band gap is mainly due to the fact that the exact functional introduced in the Hohenberg-Kohn theorem is not known. The total density of states (DOS) of undopped ZnO from LDA calculations using pseudopotential are shown in Fig. 5. The left side represents the valence band (VB) which ends at 0 eV on the fig 5.7. Actually the top of valence band is taken as 0 eV for reference purpose and the diagram is plotted. The major part of O-s and p and a small part of Zn-s and states contributes towards the VB. A combination of Zn-s and O-sp stated form the lower portion of the conduction band (CB). The total energy, the Fermi energy, the position of bands, etc., all are found to be same in both cases. The DOS plot also shows that there is no difference in the peaks and the energy gap due to relaxation which means relaxation does not cause the atoms to move away from their position and this exactly is what expected.

CONCLUSIONS

The first principle DFT calculations are done to study the structural and electronic properties of cubic ZnO. The values of different parameters like, lattice constant, band gap, band plot, charge distribution and density of states has been calculated. The findings can be summarized as follows. The description of an interacting many-particle system is, in general, very complication and approximations need to be made. Several methods in quantum physics try to describe the motion of the electrons in such systems by the electronic wave function, the solution of either the time independent or time dependent Schrodinger equation. The computational effort involved in these methods is very high. In contrast to density functional theory, the computational costs are much lower. In DFT, the electronic wave function is not evaluated for a full description of the interacting many-particles system but it is sufficient to look at the electron density. Using DFT the calculated results with the help of Quantum Espresso the results found are in good agreement with other theoretical and experimental results. The lattice constant of ZnO is calculated with energy minimization method. This value is used for further calculations. The charge density distribution is checked to know the bonding between the elements forming the compound. The band structure calculation done and band structure plotted too. The band gap was found out. It also gave us information that ZnO is an indirect band gap semiconductor. The Fermi energy for ZnOis found and the density of states is plotted. The results obtained here can be used as a basis for further investigation of properties of ZnO.

ACKNOWLEDGMENT

The authors are thankful to the lab assistant, Department of Physics and the Dean, School of Applied Sciences, Centurion University of Technology and Management, for their cooperation and motivation during this study.

REFERENCES

1. Vijaya Deshpande, A note on ancient zinc smelting in India and China. Indian journal of history of science 31.275 (1996) 275.
2. J.R Partington, A short history of chemistry, 3rd edition, Dover 1989
3. Ozgur, Y.L. Alivov, C. Liu, A. Teke, M.A. Reshchikov, S. Dogan, V. Avrutin, S.J. Cho, H. Morkoc, A comprehensive review of ZnO materials and devices, J. Appl. Phys. 98,041301(2005).
4. D.M. Bangall, Y.F Chen, Z. Zhu , T. Yao , S Koyama , M.Y. Shen, T. Goto, Optically pumped lasing of ZnO at room temperature , Appl phys. Lett. 70 (1997) 2230 – 2232
5. H. Ohno, F. Matsukura, Y. Ohno, JSAP Int. 5, 4 (2002)
6. P. Srivastava, Y. Sharma, Adv. Mat. Lett.2, 290(2011)
7. Janotti, C. G Van de walle, Rep. Prog. Phys.72 (2009) 29
8. A.B Djurisic, A.M.C Ng, X.Y. Chen, Prog. Quant.Electron.34 (2010) 191-259
9. A. Kolodziejczak-Radzimska, T .Jesionowski, Materials 7(2014) 2833 – 2881
10. Q. Fan, J. Yang, Y. Yu, J. Zhang, J. Cao, Chem. Eng. Trans. 46, 985(2015 C.E.Szakacs,E.F.MerschrodS.andK.M.Poduska,Computation1, 16 (2013)
11. D. Vanderbit, Phys. Rev.B41, 7892(1990)
12. P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. BuongiornoNardelli, M.Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carn-imeo, A. Dal Corso, S. de Gironcoli, P. Delugas, R. A. DiStasio Jr, A. Ferretti, A.Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, JJia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. K¨u¸c¨ukbenli, M .Lazzeri, M. Marsili, N.Marzari, F. Mauri, N. L. Nguyen, H.-V. Nguyen, A. Otero-de-la-Roza, L. Paulatto,S. Ponc´e, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A. P. Seitsonen, A. Smo-gunov, I. Timrov, T. Thonhauser, P. Umari, N. Vast, X. Wu, S. Baroni J.Phys.:Condens.Matter 29, 465901 (2017)
13. D. M. Ceperley and B. I. Alder, Ground State of the Electron Gas by a Stochastic Method, Phys. Rev. Lett. 45,566(1980).
14. Nonlinear ionic pseudopotentials in spin-density-functional calculations, S.G.Louie, S.Froyen, and M.L.Cohen, Phys,Rev.B 26,1738(1982).
15. Abinitio pseudopotential study of structural and high-pressure properties of SiC, K.J Chang and M.L.Cohen,P hys.Rev.Lett.35,8196(1987).
16. Self-Consistent Equations Including Exchange and Correlation Effects, W.Kohn and I.J .Sham,Phys.Rev.140,(1965)
17. Pearson's handbook of crystallographic data for intermetallic phases, P.Villars and L.D.Calvert,(ASM International,Cleveland,1991)

TABLE III comparison of the work with other experimental and theoretical result

Parameter	Calculation	Reference (Expt/Theoretical)
Lattice constant	6.3306Å	a=3.2495Å c=5.2069Å
Band gap	2.1eV	3.3 eV (direct)
Total energy	-317.46309515 Ry	Not found
Fermi energy	6.2993Ev	Not found
Charge density plot	Fig 3	In good agreement

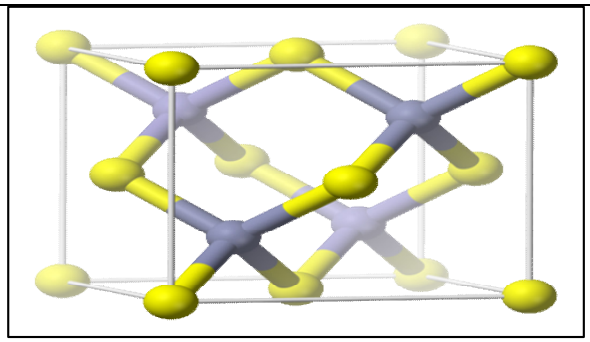

Figure 1: Hexagonal wurtzite of ZnO (yellow color is zinc graycolor is oxygen)

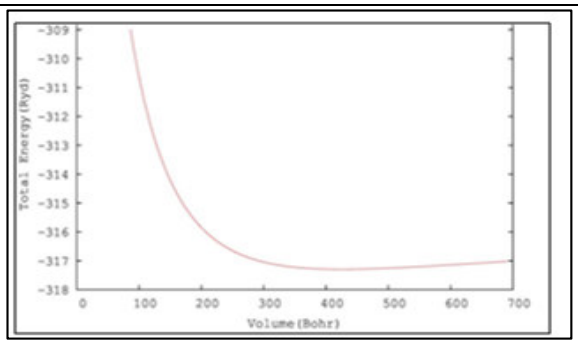

Figure 2: Plot between total energy and cell volume to determine lattice constant for ZnO

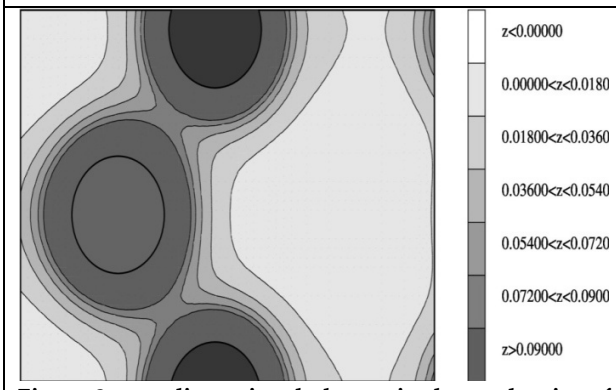

Figure 3: two dimensional electronic charge density of ZnO Electronic density of different shaded region indicated on the bar. This is the result of LDA calculation.

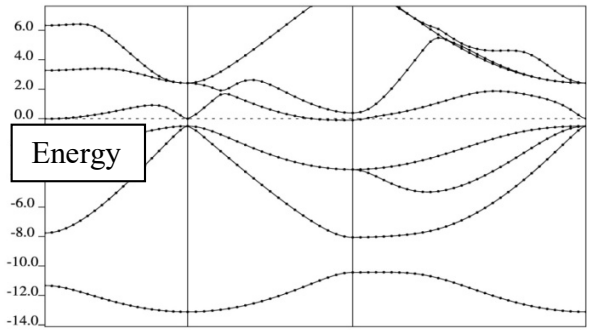

Figure 4: Band structure of ZnO at high symmetry points from PBE calculations. Symmetry points along X-axis and Energy in eV along Y-axis. Top of the valence bandis taken as zero on the energy axis. The dashed line shows the top of the valence

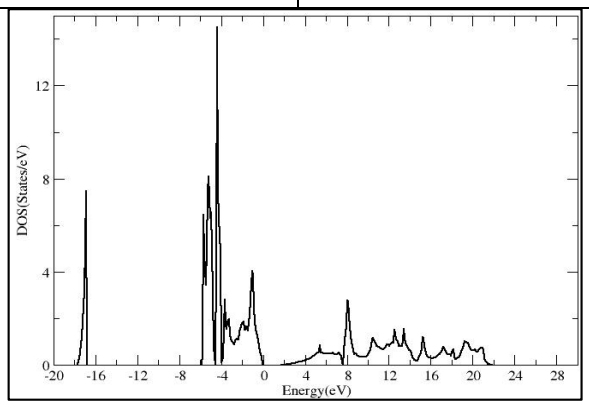

Fig 5: The total density of states of ZnO using LDA. Top of the valence band taken as 0 eV.

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RESEARCH ARTICLE

Efficient Recognition and Analysis of Epileptic Seizure Using Electroencephalogram

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ABSTRACT

The common issue in the human brain is epileptic seizure which is regularly distinguished from biopotential obtained from cerebrum as electroencephalogram(EEG). This paper emphasizes on the recognition of epilepsy utilizing Firefly Levenberg Marquardt (FLM) and Support Vector Machine (SVM). The features separated from FLM is feed to the classifier and analyzed for four surely understood grouping issues like (a) ordinary and epileptic seizure, (b) epileptic seizure and seizure free, (c) typical, epileptic seizure and seizure free and (d) epileptic seizure and non-seizure EEG signals utilizing openly accessible University of Bonn EEG information database. The exploratory reaction as far as classification accuracies have been contrasted with existing models for similar issues.

Keywords: Human brain, Epileptic, Seizure, biopotential, Data Set

INTRODUCTION

The common chronic neurological disorder in a human body is Epilepsy according to World Health Organization. So, the paroxysmal dysfunction in brain is developed by excessive neural discharge linked with some state of consciousness, recurrent and sudden malfunction of brain activity. The seizures are due to the result of transient and unexpected electrical disturbance of brain. The various investigation like Tomography, Magnetic-Resonance-Imaging (MRI), Computed-Tomography (CT Scan) and EEG are followed for detection of epilepsy. By an application of different scheme of signal processing on EEG, huge information may be extracted which are essential for proper diagnosis purposes. Most of the research work on epileptic emphases on epileptic event recognition and seizure forecast. As per survey entire 1% of world's population is affected by epilepsy and 25% can't be treated satisfactorily due to lack of skilled physician or source of care unit. As the psychological and social plays major role for epilepsy so

the life span of an individual is affected harshly. Many automated signal classification and seizure detection schemes has been applied by different researchers. A computerized system is developed for the recognition of the same [1] and using nearest-neighbor classifier on EEG feature extracted in both time and frequency domain [2] for detection of epileptic seizure. Generally, by placing EEG electrodes on different parts of brain scalp the brain activity is observed for specific diagnosis [3-5]. But the captured EEG signals from electrodes are impure as they are influenced by various unwanted signals known as artifacts. The main sources of this artifacts are improper positioning of electrode, noise in source power, muscle contraction, eye movement and environmental factors [6-8] etc. Therefore, the diagnosis of EEG signal is very complex due to presence of these artifacts. Hence, a pure EEG signal is required for proper analysis by removing the unwanted noise or artifacts in captured EEG [9] signal. In order to eliminating the artifacts, a suitable model should be developed which having low distortion of amplitude [10-11]. Various schemes commonly used by researchers for eliminating the artifacts are Independent component analysis (ICA) [12], Wavelet Transforms (WT) [13,14], Linear filtering [15,16] and cascade adaptive filter [17]. Apart from these schemes the other methods like Principal Component analysis is also used but it has some limitations like orthogonal rotation limits. The EEG signals are generally considered for detection of epilepsy, but it is very tedious in long time investigation. Hence a fast, reliable and automatic recognition of epilepsy from EEG signal can be achieved by a hybrid model [18-22] using FLM and SVM scheme. Time frequency domain and non-stationary signal decomposition scheme of epilepsy detection is also possible [29-33].

Main objective of the proposed work is to plan and develop a model for recognition and analysis of Epileptic Seizure in Electroencephalogram by removing artifacts based on FLM optimization algorithm along with neural network oriented adaptive filtering. In primary stage the captured EEG signal is feed to proposed adaptive filtering for getting optimal weights through Fire-Fly (FF) algorithm and LM (Levenberg Marquardt). This hybridized two algorithms are then applied to neural network for obtaining the optimal weights for adaptive filtering. Finally, the proposed filter is used for artifacts removal form captured EEG signal.

METHODOLOGY

Original data from the electrodes are influenced by signal contaminations or various noise sources as a result this desired signal is randomly fluctuates and unsuitable for proper diagnosis. In order to meet the desired specification, the noise or artifacts must be optimized. But the main problem for EEG artifacts removal is threshold level selection because of its uncertainty. All the biopotentials originates from the living organs are time varying in nature so the artefacts associated with the biopotentials like EEG are removed by adaptive filters in some extent. But there are some limitations for using adaptive filters because of nonlinear issues. Hence, for smooth removal of artifacts from EEG signal, an optimal weight is highly necessary for adaptive filtering which is a prime objective of the proposed work. Figure-1 represents a Schematic diagram for noise optimization is followed for artifacts removal in EEG signal. In the presented diagram, two inputs are used for the analysis. Here one input from EEG source signal E(t) and other from artifact sources Ar(t) are applied to adaptive filter for proper optimization. Before feed to adaptive filter the Artifact is applied to non-linear dynamics for generating an interference signal Int(t). Then combination of both interference and EEG signal develops a primary input signal Pr(t) and is expressed as Pr(t)=E(t)+Pr(t)

Now the Ar(t) is feed to adaptive filter for getting filtered response F(t) which is again substracted from the resultant Pr(t), expressed as O(t)=Pr(t)-F(t) [34-35]. Here O(t) represents the output of adaptive structure for noise optimization.As the acquired signal is a nonlinear so a nonlinear autoregressive exogenous model (NAREX) should be followed which is a best scheme of time series analysis. This NAREX model is comprises of multilayer feed forward network, recurrent loop and time delay as explaned in the proposed work. Again this model is contains three vector layer like input layer, hidden layer and the output layer. Here, Input layer contains three vectors like exogenous input vector, delayed regressed output vector and delayed exogenous input vector. Finally the out put

vector after completion of neural operation is developed as L(n+1). An internal structure of NAREX model is presented in figure-2 and the mathematical expression for this model is presented as [36-38].

L(n+1)=f(L(n),.....,L(n-D_L); V9n),....,V(n-DV))

In figure 3 the detailed algorithm flow chart for proposed model is presented and it contains the 5 stages where the various factors are associated for analysis. The intensity of fire fly in stage-1 is calculated as

$$I_d = \frac{I_0}{1+\lambda d^2} \quad \text{.....(1)}$$

The term I_d is the intensity of fire fly at a distance 'd'. Similarly the attractiveness is calculated as

$$A_d = \frac{A_0}{1+\lambda d^2} \quad \text{.....(2)}$$

Weighted function used in fire fly algorithm is presented as [39]

$$W_{ff}^{t+1} = W^t + A_0 e^{-\lambda d^2} (W_{cb} - W^t) + \gamma\varepsilon \quad \text{.....(3)}$$

In equation (3) λ is the absorption coefficient of light and, ε is a random number and W_{cb} is the current best solution. When firefly algorithm is applied, then bothe input vector and updated vector are comined as per the equation (4)[40].

$$O_{ff} = V(W, W_{New}) \quad \text{.....(4)}$$

Here in eqution (4) O_{ff} is the updated output, W is input vector, W_{New} is the new weighted vector developed from fire fly algorithm.

The block diagram shown in figure 4 is suitable and fully functional unit for recognition and classification of epileptic sezure in EEG. As per the above explaination the EEG signal is preprocessed by an application of FLM algorithm and now the processed signal containing valuable information is used for extracting the various features for data set formation. Then after a trained data sets are formed for proper classifcation in terms of seizure, Normal and seizure free EEG signal. Here the SVM with Radial-Basis-Function (RBF) is used with a trade off parameter and sigma parameter are 2.289 and 0.11 respectively.

RESULT AND DİSCUSSİON

The proposed model uses real signal which is obtened from the Bonn University toolkit for carried out performance analysis. This data set contains an EEG signal of a healthy person and it is free from seizure activity. The EEG recordings of a healthy person is achieved by the action or condition of eye state like open or closed denoted by Z and O. Each subsets in data set has 100 Eeg signals of seizure free. Similarly during seizure activity the subst data set is N and F . For evaluation of performance, the four problems are considered like normal (N) with epileptic seizure (ES), Seizure free (SF), Non Seizure (NS). The ES is observed during the Subset of S, SF is obtained at N and F subsets and NS is available at Z,O,N. A sample EEG signals of various states are presented in Figure-5 (a,b,and c)

The plot of accuracy,sensitivity and specificity is given as follows:
This projected techniques is executed with MatLab by considering the real signals obtained from the aforsaid database. The interval for the signals to be analysed is fixed at one minutes and by adding external unwanted signal as artefacts for required analysis. Again the acquired bio-signals are sampled at 256 samples per second with a 16 bit resolution. Table-1 indicates the performance analysis of four classification problems as in terms of Accuracy (ACC),

Sensitivity (SEN) and Specificity (SPEC). Similarly table 2 depicts the perfromance comparision of the proposed scheme with the other existing scheme in terms of accuracy and it is concluded that the proposed scheme projected the better response than the others. During experimentation several techniques like Independent Component Analysis (ICA), Wavelet Transform Analysis (WTA), Neural Network along with LM and the proposed NARX neural networks are considered for artefacts removal and feature extraction. Hence the table 3 outlined the performance analysis in terms of signal to noise ratio (SNR), Root Mean Square Error (RMSE) amd Mean Square Error.

CONCLUSION

This paper proposed a proficient model for the prediction of epilepsy from the EEG signal. The technique has been examined for four comprehended issues specifically, normal and epileptic seizure, epileptic seizure and seizure free, epileptic seizure and non-seizure, normal epileptic seizure, and seizure free classes of EEG signals. The performance of the proposed method has been compared with the current classification techniques. Therefore the proposed model has reliable improvement in gathering accuracy over the conventional procedure. In like way, the proposed model is moreover giving the satisfactorily high classification accuracy in various portion of the EEG signal.

REFERENCES

1. Reddy, G. Ravi Shankar, and Rameshwar Rao. "Automated identification system for seizure EEG signals using tunable-Q wavelet transform." Engineering science and technology, an international journal, Elsevier,20.5 (2017): 1486-1493.
2. Sharma, Rishi Raj, and Ram Bilas Pachori. "Time–frequency representation using IEVDHM–HT with application to classification of epileptic EEG signals." IET Science, Measurement & Technology 12.1 (2017): 72-82.
3. Sharma, Rajeev, and Ram Bilas Pachori. "Classification of epileptic seizures in EEG signals based on phase space representation of intrinsic mode functions." Expert Systems with Applications, Elsevier, 42.3 (2015): 1106-1117.
4. Zhu, Guohun, Yan Li, and Peng Paul Wen. "Epileptic seizure detection in EEGs signals using a fast-weighted horizontal visibility algorithm." Computer methods and programs in biomedicine 115.2 (2014): 64-75.
5. Ahammad, Nabeel, Thasneem Fathima, and Paul Joseph. "Detection of epileptic seizure event and onset using EEG." BioMed research international 2014 (2014).
6. Azar, Ahmad Taher, and Shaimaa Ahmed El-Said. "Performance analysis of support vector machines classifiers in breast cancer mammography recognition." Neural Computing and Applications 24.5 (2014): 1163-1177.
7. Fu, Kai, et al. "Classification of seizure based on the time-frequency image of EEG signals using HHT and SVM." Biomedical Signal Processing and Control 13 (2014): 15-22.
8. Lee, Sang-Hong, et al. "Classification of normal and epileptic seizure EEG signals using wavelet transform, phase-space reconstruction, and Euclidean distance." Computer methods and programs in biomedicine 116.1 (2014): 10-25.
9. Joshi, Varun, Ram Bilas Pachori, and Antony Vijesh. "Classification of ictal and seizure-free EEG signals using fractional linear prediction." Biomedical Signal Processing and Control 9 (2014): 1-5
10. Fu, Kai, et al. "Classification of seizure based on the time-frequency image of EEG signals using HHT and SVM." Biomedical Signal Processing and Control, Elsevier, 13 (2014): 15-22.
11. Parey, Anand, and Ram Bilas Pachori. "Gear fault diagnosis based on central tendency measure of intrinsic mode functions", International Journal of COMADEM 17.3 (2014): 15-22
12. Pachori, Ram Bilas, and Shivnarayan Patidar. "Epileptic seizure classification in EEG signals using second-order difference plot of intrinsic mode functions." Computer methods and programs in biomedicine 113.2 (2014): 494-502.

13. Patidar, Shivnarayan, and Ram Bilas Pachori. "Classification of cardiac sound signals using constrained tunable-Q wavelet transform." Expert Systems with Applications 41.16 (2014): 7161-7170.
14. Sharma, Rajeev, Ram Bilas Pachori, and Shreya Gautam. "Empirical mode decomposition-based classification of focal and non-focal seizure EEG signals." Medical Biometrics, 2014 International Conference on. IEEE, 2014.
15. Acharya, U. Rajendra, et al. "Automated EEG analysis of epilepsy: a review." Knowledge-Based Systems 45 (2013): 147-165.
16. Bajaj, Varun, and Ram Bilas Pachori. "Epileptic seizure detection based on the instantaneous area of analytic intrinsic mode functions of EEG signals." Biomedical Engineering Letters 3.1 (2013): 17-21.
17. Acharya, U. Rajendra, et al. "Automated EEG analysis of epilepsy: a review." Knowledge-Based Systems 45 (2013): 147-165.
18. Li, Shufang, et al. "Feature extraction and recognition of ictal EEG using EMD and SVM." Computers in biology and medicine 43.7 (2013): 807-816.
19. Uthayakumar, R., and D. Easwaramoorthy. "Epileptic seizure detection in EEG signals using multifractal analysis and wavelet transform." Fractals 21.02 (2013): 1350011.
20. Tzallas, Alexandros T., et al. "Automated epileptic seizure detection methods: a review study." Epilepsy-histological, electroencephalographic and psychological aspects. InTech, 2012.
21. Nicolaou, Nicoletta, and Julius Georgiou. "Detection of epileptic electroencephalogram based on permutation entropy and support vector machines." Expert Systems with Applications 39.1 (2012): 202-209.
22. Bajaj, Varun, and Ram Bilas Pachori. "Classification of seizure and nonseizure EEG signals using empirical mode decomposition." IEEE Transactions on Information Technology in Biomedicine 16.6 (2012): 1135-1142.
23. Pal, Saurabh, and MadhuchhandaMitra. "Empirical mode decomposition-based ECG enhancement and QRS detection." Computers in biology and medicine 42.1 (2012): 83-92.
24. Parey, Anand, and Ram Bilas Pachori. "Variable cosine windowing of intrinsic mode functions: Application to gear fault diagnosis." Measurement 45.3 (2012): 415-426.
25. Bajaj, Varun, and Ram Bilas Pachori. "Classification of seizure and nonseizure EEG signals using empirical mode decomposition." IEEE Transactions on Information Technology in Biomedicine 16.6 (2012): 1135-1142.
26. Park, Yun, et al. "Seizure prediction with spectral power of EEG using cost-sensitive support vector machines." Epilepsia 52.10 (2011): 1761-1770.
27. Oweis, Rami J., and Enas W. Abdulhay. "Seizure classification in EEG signals utilizing Hilbert-Huang transform." Biomedical engineering online 10.1 (2011): 38.
28. Pachori, Ram Bilas, and Varun Bajaj. "Analysis of normal and epileptic seizure EEG signals using empirical mode decomposition." Computer methods and programs in biomedicine 104.3 (2011): 373-381.
29. Acharya, U. Rajendra, S. VinithaSree, and Jasjit S. Suri. "Automatic detection of epileptic EEG signals using higher order cumulant features." International journal of neural systems 21.05 (2011): 403-414.
30. Acharya, U. Rajendra, et al. "Application of recurrence quantification analysis for the automated identification of epileptic EEG signals." International journal of neural systems 21.03 (2011): 199-211.
31. Temko, A., et al. "EEG-based neonatal seizure detection with support vector machines." Clinical Neurophysiology 122.3 (2011): 464-473.
32. Zavar, M., et al. "Evolutionary model selection in a wavelet-based support vector machine for automated seizure detection." Expert Systems with Applications 38.9 (2011): 10751-10758.
33. Li, Yan, and Peng Paul Wen. "Clustering technique-based least square support vector machine for EEG signal classification." Computer methods and programs in biomedicine 104.3 (2011): 358-372.
34. Übeyli, ElifDerya. "Lyapunov exponents/probabilistic neural networks for analysis of EEG signals." Expert Systems with Applications 37.2 (2010): 985-992.
35. Guo, Ling, Daniel Rivero, and Alejandro Pazos. "Epileptic seizure detection using multiwavelet transform based approximate entropy and artificial neural networks." Journal of neuroscience methods 193.1 (2010): 156-163.
36. Altunay, Semih, ZiyaTelatar, and Osman Erogul. "Epileptic EEG detection using the linear prediction error energy." Expert Systems with Applications 37.8 (2010): 5661-5665.

37. Freund, R. J., Wilson, W. J., & Mohr, D. L. (2010). Statistical methods (3rd ed.). Burlington, MA, USA: Academic Press.
38. Liang, Sheng-Fu, Hsu-Chuan Wang, and Wan-Lin Chang. "Combination of EEG complexity and spectral analysis for epilepsy diagnosis and seizure detection." EURASIP Journal on Advances in Signal Processing 2010 (2010): 62.
39. Altunay, Semih, ZiyaTelatar, and Osman Erogul. "Epileptic EEG detection using the linear prediction error energy." Expert Systems with Applications, Elsevier, 37.8 (2010): 5661-5665.
40. Ghosh-Dastidar, Samanwoy, HojjatAdeli, and Nahid Dadmehr. "Principal component analysis-enhanced cosine radial basis function neural network for robust epilepsy and seizure detection." IEEE Transactions on Biomedical Engineering 55.2 (2008): 512-518.
41. Adeli, Hojjat, Samanwoy Ghosh-Dastidar, and Nahid Dadmehr. "A wavelet-chaos methodology for analysis of EEGs and EEG subbands to detect seizure and epilepsy." IEEE Transactions on Biomedical Engineering 54.2 (2007): 205-211.
42. Swami, P., Gandhi, T.K., Panigrahi, B.K., et al.: 'A novel robust diagnostic model to detect seizures in electroencephalography', Expert Syst. Appl., 2016, 56, pp. 116–130
43. Tiwari, A.K., Pachori, R.B., Kanhangad, V., et al.: 'Automated diagnosis of epilepsy using key-point-based local binary pattern of EEG signals', IEEE J. Biomed. Health Inf., 2017, 21, (4), pp. 888–896
44. Li, Y., Wang, X., Luo, L., et al.: 'Epileptic seizure classification of EEGs using time–frequency analysis based multiscale radial basis functions', IEEE J. Biomed. Health Inf., 2017, DOI: 0.1109/JBHI.2017.2654479

Table 1: Performance analysis of various classifcation stage

Classification	ACC	SEN	SPEC
ZOS	99.9	99.9	99.9
NFS	98.44	98.24	98.12
ZONFS	97.21	97.42	97.32
ZO-NF-S	97.87	97.21	97.02

Table 2: Performance analysis of proposed model with existing model

Sl. No.	Ref. No.	Methods	Accuracy	Sensitivity	Specificity
1	[2]	Nearest neighbor classifier (IEVDHM-HT)	99.67	99	100
2	[10]	HHT AND SVM	99.125	NA	NA
4	[12]	ICA	97.75	97.68	98.07
5	[13,14]	WT	99.42	--	--
6	[16]	Linear filtering	89.81	90	89.31
7	[42]	dual tree complex WT, energy, standard deviation etc. and neural network classifier	98.67	99	98.54
8	[18]	EMD and SVM	--	93.25	96.90
9	[43]	key-point local binary pattern and LS-SVM	99.45	99.68	99

		classifier			
10	[21]	Permutation entropy and SVM	--	94.38	93.23
11	[44]	TF analysis, TVAR model, and multiscale RBF	98.73	98	99.10
12	[27]	Hilbert Huang transform	97.72	--	--
13	Proposed method	FLM-SVM	99.72	99.18	100

Table3 : Performance Analysis

Schemes	SNR	RMSE	MSE
Proposed FLM	43.025	0.12025	4421
Cascade Filter	38.325	18.9852	50214.4
WTA	12.236	63.2966	53210.5
ICA	8.7528	67.2587	5407.6
NN-LM	43.012	0.210221	4236.4

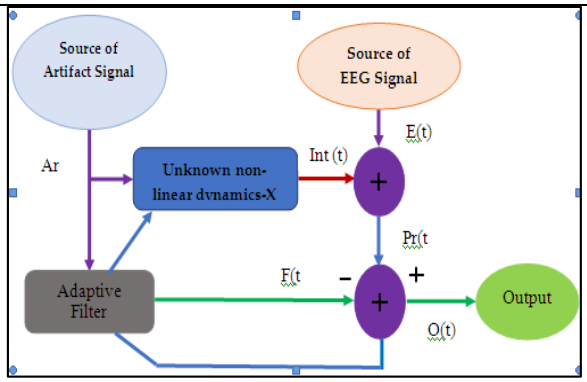

Figure 1: Schematic diagram for noise optimization

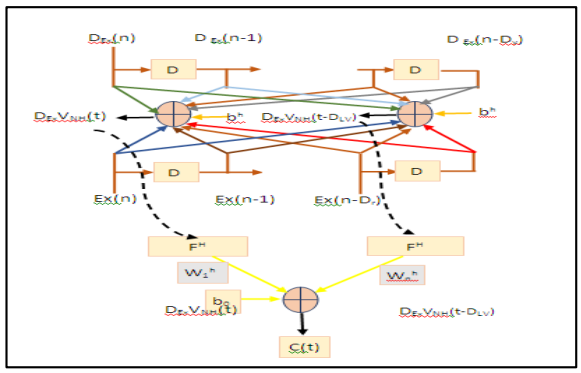

Figure 2(a) Internal structure of Nonlinear Autoregressive Exogenous model (NAREX)

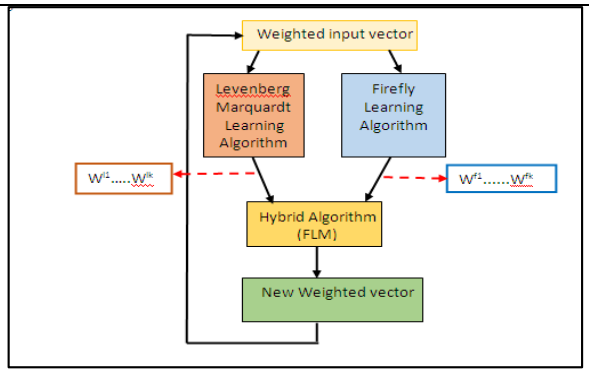

Figure 2: (b) Proposed hybrid optimization scheme

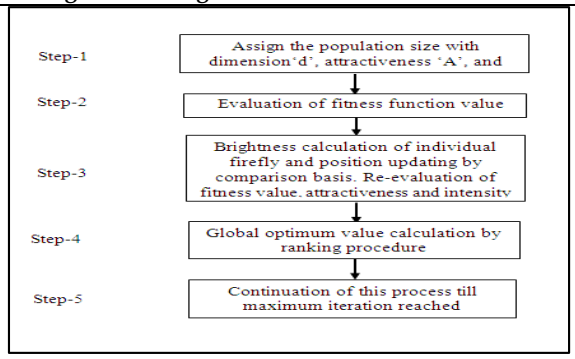

Figure 3 : Detailed algorithm flow chart for proposed hybrid model

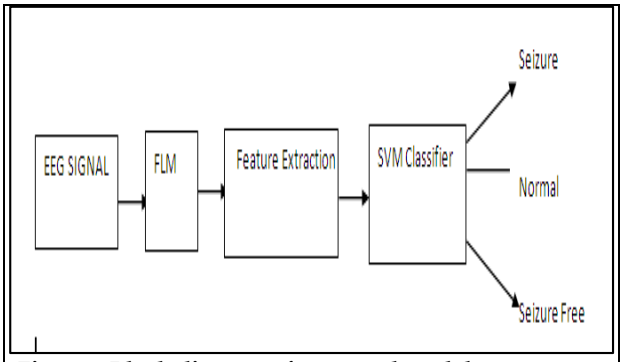

Figure:4 Block diagram of proposed model

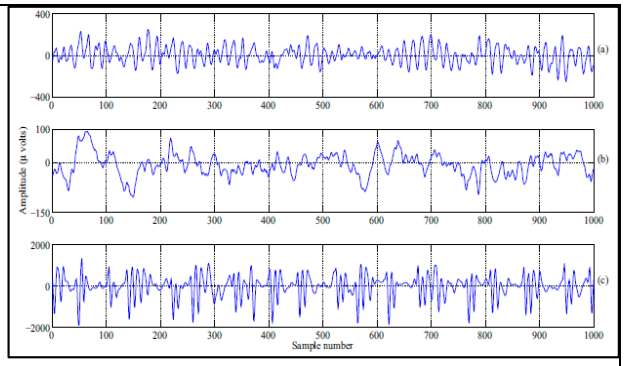

Figure:5: Various state of EEG signal considering (a) Normal, (b) Seizure free and (c) epileptic seizure

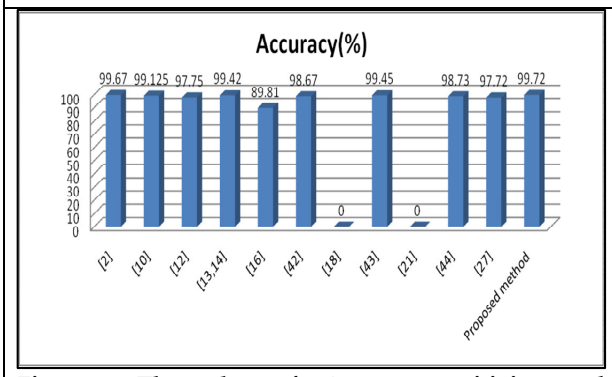

Figure:6: The plot of Accuracy,sensitivity and specificity of the proposed model compared with others (a) Accuracy

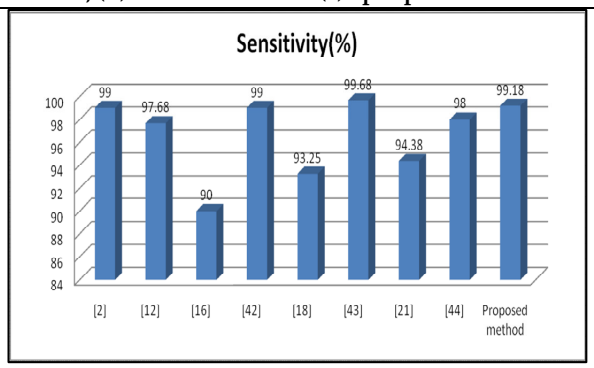

Figure:6: The plot of Accuracy,sensitivity and specificity of the proposed model compared with others (b)Sensitivity

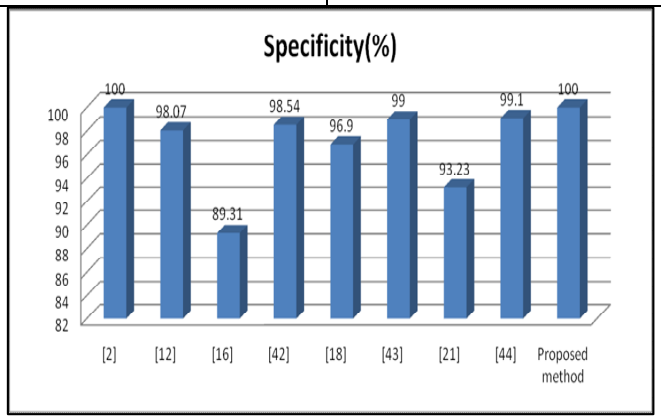

Figure:6: The plot of Accuracy,sensitivity and specificity of the proposed model compared with others (c) Specificity

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RESEARCH ARTICLE

Future of Drone Technology in India

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ABSTRACT

This paper gives an overview about the future of drone technology in India. For the development of the society in every aspect, new technologies need to be adopted. Starting from agriculture to military applications, everywhere, new technologies are implemented to increase their work capability efficiently. Human being can work limited hours per day whereas the machines with advanced technology can work 24 hours per day which helps for the increase in productivity. The drone technology is one of the emerging technologies which is rapidly increasing in the whole world. It is basically an unmanned vehicle which can fly in the sky and controlled remotely from the ground. So risk factor on human life is negligible. Anyone can transfer any objects from one place to another without taking much more time and it doesn't depends on traditional courier systems. Drone technology has many applications and due to its low cost, everyone can avail it. In India, its popularity is increasing day by day and people are accepting this as it doesn't require any advanced training to operate it. It operation is so simple that people can control it by using mobile app. A through survey has done about the various usability of drones and what it its future in Indian market. The different parts and technology involved in the drones are explained. The different rules and regulations provided by government of India regarding the use of drones are also explained. The various potential manufacturers which are already established their market in India are provided. The areas which are not explored and how drone technology can be implemented there also discussed here.

Keywords: Technology, Industry, Unmanned Aerial Vehicle (UAV), Drone

INTRODUCTION

The technological advancement and its use in day to day activities have made the human life easier. In every field, the human being alone can't able to achieve the goal without the support of technology. The technologies are implemented in various sectors like health, education, automobiles industries, all types of manufacturing industries,

emergency services, agriculture, engineering services, entertainment industry, military applications, energy industry, e-commerce, weather forecasting, environmental monitoring and so on [1]. As the human needs increases, the approach to the technology also changes. In the busy life of today's society, people try to minimise the time effect and wants more work to be done with short period of time which helps in economic growth [2]. It is impossible for the human being to deliver the services at multiple places. To overcome this, various technologies are used which reduces the time burden. The drone technology is one of them which recently adopted by various service sectors to fulfil the target easily and effectively. Usually, the drone also called as the unmanned aerial vehicle (UAV) which can fly in the sky is remotely controlled by the ground operator with the help of controller and communication systems [3]. The energy storage i.e. battery is the main source of energy to drive the drone. The solar energy is also one of the power source which is used to enhance its driving duration. The first UAV is used in 1849 which is officially registered. By seeing their popularity and with the development in technology, the updated and more efficient UAV are gradually developed. Today's UAV uses artificial intelligence (AI) technology which provides excellent performance in wider applications. There are different types of drones are available based on their applications and their performances. In each and every sector, it is going to be the necessary to get a position in this competitive world. It can be used both in commercial sector and also for personal use. It helps in various industries to increase the productivity, reduces the work load, strengthen the customer relations, and increase the work efficiency [4]. The technology is so advance that it can be controlled and monitored by mobile app. Due to less expensive, the small industries can invest money on it to get a higher profit and can connect to the customers easily and efficiently. This papers explains about the various types of drones and its components. A detailed list of drone manufacturing company in India is provided. The various application areas of drone are explained and how the use of it in India can be maximized is explained.

LITERATURE REVIEW

Drone technology is an emerging technology in the field of aviation. Its uses started from World War I and now it is one of the leading industries. There are different classifications of drones which are available in the market and can be differentiated in terms of the type, size, weight, power source and the degree of autonomy [5]. The drone specifications are important for its range, duration of flight, and the loading capacity. The drone needs wireless communications for control with an operator on the ground. In drone there are different system used such as fixed-wing systems, multirotor systems and other systems such as hybrid systems, ornithopters drones that use turbo fans. There are different technologies used to keep the drone flying which helps to defines the drone types. The drone characteristic is one of the determining factor in the shape level of autonomy and appearance of the drone. The autonomy of a drone can vary from full autonomous operation to fully control by a remote pilot. The size of a drone varies from the small size like an insect to the big size like a commercial airplane. Its weight varies from milligrams to kilograms. The main characteristic is its different source of energies like battery cells, solar cells etc.

An example of a drone is shown in Fig.1. There are various components used in a drone. Those components are dc motor and its controller, battery for its power, propellers, power distribution unit, flight controller and its sensor, transceiver, camera and memory card [6]. The motor is used to rotate the propellers. The electronics speed controller is required for the motor so that the drone movement can be controlled. The dc motor requires the dc power where battery helps to supply that power. The advanced rechargeable Li-ion battery is used and it can be charged during flight also with the help of solar cells mounted on the drone. The motor helps to rotate the propeller which converts rotational motion into thrust helps to move the drone. The different electronic components used in drone require power where power distribution unit helps to supply power to them. The drone motion, height and range are needed to be controlled with the help of fight controller and its sensor. The transceiver is required for the controller to send and receive the commands. The camera is also required for the different observations. The videos are stored in a memory card.

Applications of Drone

The drone is used in various applications such as aerial photography, e-commerce shipping and delivery, geographical mapping, disaster management control, precision agriculture, search and rescue, weather forecast, wildlife monitoring, law enforcement, entertainment, public safety, civil security, traffic and crowd management, various types of surveys, data generation and so on. There is no limitation of using this technology. Drone photography is one the interesting photography which gives beautiful images from the sky. Now a day in every occasion, photographers are using drone to take videos and photos. In e-commerce, for delivering and shipping, drones are used. So you can get anything in the same day delivery and there is fear of traffics. You can get you order within time. For geographical mapping, the use of drone is widely accepted. It makes the job easier and takes very less time for it. To control and monitor of any disaster, it is used. In such time, the area and location may not be accessible by person. It helps to locate the life which is in danger. In case of farming, drones are used for inspection of plants, thermal imaging, spreading of waters and pesticides which help in the increase of crop production. For search and rescue of life, it helps a lot during any unusual situation. In military applications also, it is used to prevent any unwanted event. In 2014, India had imposed ban on the use of civil drones. By looking into so many applications, in 2018, the government of India has removed the restrictions about its use and came up with some regulatory policies. But still some area wise restrictions are there because of safety issues. Indians can fly the drone in India but foreigners are not allowed to use it in India.

Drone laws in India come under Ministry of Civil Aviation. The government gives some guidelines for flying a drone in India [7-9]. Those are

- All Drones except those in the Nano category must be registered and issued a Unique Identification Number (UIN).
- GPS, return to home facility, anti-collision light, ID plate, flight controller with flight data logging capability, RFID technology must be included except Nano Drone.
- A permit is required for commercial drone operations (except for those in the Nano category flown below 50 feet and those in the Micro category flown below 200 feet).
- The pilot of Drone must maintain a direct visual line of sight at all times while flying.
- Drones are not allowed to flow more than 400 feet vertically.
- No Fly Zones is defined for the Drones where no drones are allowed in that area. Those areas are airports, international borders, Vijay Chowk in Delhi, State Secretariat Complex in State Capitals, strategic locations, and military installations.
- It is mandatory to take permission to fly the drone which can be obtained by filing a flight plan and obtaining a unique Air Defense Clearance (ADC)/Flight Information Center (FIC) number.

The drones are categorized based on their weight such as:

- Nano Drone: ≤ 250 grams.
- Micro Drone: 250 grams to 2kg.
- Small: 2kg to 25kg.
- Medium: 25kg to 150kg.
- Large: > 150kg.

Till March 2020, the Ministry of Civil Aviation (MOCA) has registered 19,553 for fly in Indian sky.

Drone Industry in India

By looking into Indian market, a lot of company has stated for manufacturing the drone. Till now, around more the 40 manufactures are making drone in India [10]. Some of them are explained.

Aarav Unmanned Systems

This manufacturer started in Bengaluru in 2013. It is specialized in image processing, 3D mapping and precision agriculture.

Cron Systems
This manufacturer started in New Delhi in 2016. It is a border defence manufacturer. Cron leverages IoT technology in building intrusion detection systems.

Detect Technology
This company has started in 2014 in Chennai. A completely automated remote control system is developed and manufactured by this company. It raised $3.30 Mn Series A from SAIF Partners, Bharat Fund and others.

Drones Tech Lab
It started manufacturing in 2016 in Kolkata. It handles both manufacturer and distributor of surveillance drones and drone camera.

Idea Forge
It started its manufacturing in 2007 in Mumbai. It designs and develops its own drone. Its main focus is on surveillance and security based drone. This drone manufacturer is one of the oldest startups in India.

Indrones Solution
It is also a Mumbai-based drone manufacturer. It focuses on aerial photography and videography and based on the demand, it customises its own product.

Indshine
This startup company started in 2016 in Gurugram. This company focuses on visualisation in 2D and 3D in online platform.

Pigeon Innovative Solutions
This company started in Mumbai in 2016. Its drone focuses on aerial photography. It is specialized in the areas of surveying, 3D models, drone inspection etc.

Quidich Innovation Labs
This company started in Mumbai in 2015.It uses drones for developing end products and customises the based on the clients demand.

Redwing Aerospace Laboratories
It is started in Bengaluru in 2018. Its drone technology focuses on the application of data analytics and aerial robotics.

Skylark Drones
It is started in Bengaluru in 2014. It is a solutions provider for the drone applications. It provides solutions to improve productivity, safety for the mining, infrastructure and utilities.

TechEagle Innovations
It is started in Lucknow in 2017. It focuses on developing drones for last-mile delivery. Zomato has taken this company in December 2019.

Thanos Technologies
It is started in Hyderabad in 2016. This startup company provides drones for the application of aerial surveys and geographical mapping.

The ePlane Company
Chennai-based ePlane Company leverages its deeptech platform to provide industrial drone solutions.

Vizzbee Robotic Solutions
This startup company is started in in 2008. This company is oriented to provide solutions to autonomous section which helps in search and rescue missions in areas where it is difficult to for human being.

CONCLUSION

The future of drone technology in India is explained in this paper. Its use in different applications is explained. The components required to develop a drone is explained. The rules and regulations provided by government of India are provided. A list of different statup companies in India is provided. It is an emerging technology which takes the whole market because of its usability. A further study is required to improve its range and duration of flight time.

The advanced battery technology need to be used and other source of power need to be studied which can further enhance its use.

REFERENCES

1. H. Thohari, P. Ayu, T. Indria and Sueb, "The Development of Technology for Human Civilization", Third Basic Science International Conference, pp. 1-5,2013
2. Naikoo, S. Thakur, T. Guroo, and A. Altaf, "Development of Society under the Modern Technology - A Review", Scholedge international journal of business policy and governance, vol. 5, issue 1, pp. 1-8, 2018.
3. https://en.wikipedia.org/wiki/Unmanned_aerial_vehicle
4. https://www.businessinsider.in/tech/news/drone-technology-uses-and-applications-for-commercial-industrial-and-military-drones-in-2020-and-the-future/articleshow/72874958.cms
5. B. Vergouw, H. Nagel, G. Bondt and B. Custers, "Drone Technology: Types, Payloads, Applications, Frequency Spectrum Issues and Future Developments", Book Chapter 2, T.M.C. Asser press, 2016.
6. Saurav Kumar and E.Kanniga, "Literature Survey On Unmanned Aerial Vehicle", International Journal of Pure and Applied Mathematics, vol. 119 no. 12, 2018.
7. https://uavcoach.com/drone-laws-in-india/
8. https://inc42.com/datalab/lagging-drone-policy-in-india-leaves-commercial-drone-usage-in-limbo/
9. https://www.allerin.com/blog/10-stunning-applications-of-drone-technology
10. https://inc42.com/features/these-15-drone-startups-are-flying-high-in-indias-digital-sky/

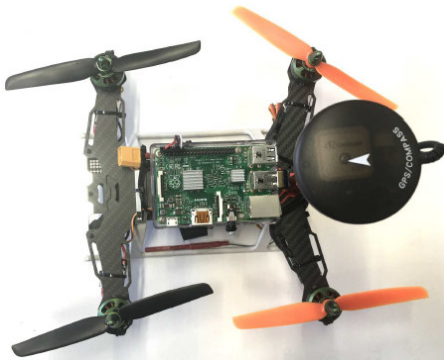

Fig. 1 Example of a drone.

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RESEARCH ARTICLE

Impact of the Pan India Lights OFF on Indian Electricity Grid on 5th April 2020

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ABSTRACT

This paper presents a study on Indian electricity grid during Pan India lights off on 5th April 2020. A study on power grid behaviour is performed and impacts of power and frequency variations are analyzed. The different power generating stations like hydro, thermal, gas, solar, wind etc. fulfil the total power demand. The load dispatch centre helps to manage the power distribution all over the India. The electrical load always varies throughout the day. Sometimes, the load demand is on the peak where more generation of electrical power is required. Similarly when the power demand is very low some generating stations need to be shut down to avoid the surplus power. On 5th April 2020, to reduce the effect of COVID-19 it has been instructed to switch OFF all the light loads from 9 PM to 9.09 PM all over India. So, in that time period there is a huge reduction in power demand which needs to be taken care at the generating stations to stabilize the grid voltage and frequency within the limits. During this time period, the different behaviour of the grid has been analyzed and provided in this paper. The grid behaviour on 5th April 2020 is compared with previous day grid behaviour. The load dispatch centres of different regions have managed the power flow by controlling the power generations.

Keywords: Power Grid, Power Demand, Power Stability, SLDC, POSOCO, NLDC, REC.

INTRODUCTION

The total electricity consumed by households to run various electrical appliances like LED bulbs, ceiling fans, T.V., refrigerators, washing machine, grinders etc. are called Residential Electricity Consumption(REC) [11]. In case if someone turns ON any one of the electrical appliance (keeping all other loads constant), a power plant in somewhere must increase its generation capacity slightly to mitigate this increase in load demand. Fortunately for better

management of power grid system and a large number of electricity users, India is geographically divided into five regions namely, Northern, Eastern, Western North Eastern and Southern grids. Hence a small increase in load at some places can be easily balanced by significant decrease in load at some other places or small increase in generation in parts of the regions. But the gross demand across India changes significantly all over the day and years. The consumers require their small or large block of power according to their demands of their activities. Thus the load demand of one consumer at any time may be different from that of the other consumer. This results in the variation of the load on the power station from time to time [12]. In this paper, the authors are analyzing the impact of the Pan India lights out event on Indian electricity grid operation on 5th April 2020. Actually Installed capacity of India as on 28th February, 2020 is 370 GW, out of which 230 GW from Thermal, 45.6 GW from Hydro, 6.7 GW from Nuclear and 87 GW from renewable [5]. According to Indian Grid load analysis from 15th March, 2020 to 5th March, 2020 India has probably 150 GW average demands on weekdays and 140 GW on weekends during the month of March. On Sunday 15th March, 2020 average demand of India was 139.125 GW whereas it declined to 126.45 GW on 22nd March (Janta Curfew, special lock-down day). On 22nd March, Indian grid faced dip in average of 13 GW, had seen around 10% reduction in the power demand as compared to 15th March 2020 for different hours of the day. And the complete lock-down starts from 25th March, 12:00 A.M. All India electrical energy consumption reduced by nearly 300 GWH and the peak demand suppressed nearly by 20GW. The energy consumption during the lock-down period is decreased by 20-30% compared to normal day [6]. From the demand pattern of 29th March, 2020(Sunday), it has been observed that Indian power demand was around 101207 MW at 18:07 o' clock and subsequently it has been increased up to 112551 MW at 21:00 o' clock during evening peak. Therefore, considering the load behavior, it is anticipated that lighting load of household consumers may be the difference of all India power demand at 18:07 and 21:00hrs i.e, 11344 MW. Further a separate exercise has been carried out to find the total demand reduction at the grid level based on the number of household consumers in India. The calculated total reduction in demand which is reflected at grid level is 12452 MW. It was predicted from the Power System Operation Corporation Limited (POSOCO) that, switching lights OFF event will suddenly reduce the Indian power demand by 12.9 GW by analyzing the domestic lighting load [9]. It has been anticipated that there would be reduction of 12-14 GW from the lighting load. It was also predicted that it would happen in 2-4 minutes and will recover in nine minutes later within 2-4 minutes. The sharp reduction in load and subsequent recovery, which is precedented, will need to be handled through hydro and gas resources. It was being suggested that, all the hydro generation will be reduced and conserved for providing flexibility during the lighting-out event. The Thermal and gas should be scheduled to meet the load. By 20:55 hours, all the thermal generations should be reduced by 60% and hydro generations should be ramp up to meet the demand. Hydro and gas generation shall be ramped down from 20:57 hrs. The hydro generators should be kept rolling at 0-10% of the rating with discontinue. Ramping up off thermal generator shall be carried out at 21:05 hrs. Further from 21:09 hrs hydro should ramp up to meet the demand. It was also planned that, all India grid frequency should be maintained at lower frequency at 49.90 Hz from 20:30 hrs and maintained at 50.05 Hz at around 21:09 hrs due to anticipated drop in frequency and restoration of load. To keep the voltage in control, POSOCO advised that, all reactors should put in service, latest by 20:00 hrs. STATCOMS and SVCs shall be in voltage control mode with reference to voltage of 400 KV and capacitors at distribution level to be kept OFF to maintain the voltage at its nominal value. All thermal and hydro machines would absorb/generate reactive power as per capability curve. In this way, the event was managed smoothly without any untoward incident while power system parameters were maintained within limits.

LITERATURE REVIEW

We must end the darkness and uncertainty emanating from the crisis, by progressing towards light and certainty. We must defeat the deep darkness of the crisis, by spreading the glory of light in all four directions. Actually, the Hon'ble Prime Minister of India appealed to the citizens on 3rd April, 2020 at 09:10 hrs to switch OFF their lights and light lamps/ candles on 5th April, 2020 at 21:00 hrs for 9 minutes. Anticipating the Power grid collapse all across India because of sudden 9 minutes light out, the Hon'ble Minister of State for Power (I/C) later clarified only to

switch OFF the lights. After the light out event, it was observed that the total reduction in all India power demand recorded during the event was 31089 MW. All India power demand started reducing from 20:45 hrs and minimum demand of 85,799 MW was recorded at 21:10 hrs. Subsequently, from 21:10 hrs, the demand started picking up and settled around 114400 MW at 22:10 hrs. At the same time, grid frequency during the event remained in the range of 50.26 Hz to 49.70 Hz with maximum and minimum frequency of 50.259 Hz and 49.707 Hz recorded at 21:08 hrs and 20:49 hrs, respectively. During this period, hydro generation across the country was maximized by 20:45 hrs and generation reduction of 17543 MW (from 25559 MW to 8016 MW) between 20:45 hrs to 21:10 hrs (matching with demand reduction of 31089 MW during the same period) was achieved with these resources. This hydro generation was again increased from 8016 MW to 19012 MW from 21:10 hrs to 21:27 hrs to meet the increase in demand after the event. Reduction of total 10950 MW generation was achieved through Thermal (6992 MW), Gas (1951 MW) and Wind generation (2007 MW) during 20:45 hrs to 21:10 hrs. In order to keep voltages and line loadings within permissible limits, some advance actions such as switching OFF transmission lines, taking reactors in service, changing SVC, STATCOM, HVDC set points etc. were taken prior to the event [10]. Since power system parameters were maintained within the limits during this 9 minutes interval, this unprecedented challenge was managed smoothly without any disturbances.

All India Power and Frequency Demand

The Fig. 1 shows the All India Power demand of two days i.e. 4th and 5th April, 2020 between the time period of 20 hrs 30mins to 21 hrs.45 mins. It is observed that on 4th April, 2020, power demand is almost constant i.e. around 12000 MW throughout the mentioned time period. But on 5th April, 2020 and same time period, there is a huge drop of power demand for a certain period of time. Power falls slowly at time of 20hr:30 mins and around at time of 20:55 o'clock, it suddenly falls. It falls from 11500 MW to around 8600 MW. This remains around for 5 mins and then starts increasingly slowly. At the time of around 21:45 o'clock, the power demands returns to its actual position.

The Fig. 2 shows the All India Frequency Variation on 5th April, 2020 between the time period of 20 hrs 30mins to 21 hrs.45 mins. It is observed that on 5th April 2020 frequency which starts at 50 Hz at 20 hrs 29 mins, suddenly falls to 49.7 Hz around 20 hrs 49 mins and after that it starts increasing and finally reaches at 50.25 Hz at 21 hrs 04 mins because of light out event.

Region wise details of Expected Load Reduction

As per the data received from SLDC, it is inferred that total reduction in domestic lighting load on all India level is anticipated to be 12 – 14 GW. This reduction in load occurs in 2-4 minutes and after 9 minutes it will again be recovered within 2-4 minutes. This sharp reduction in load and subsequent recovery need to be handled carefully by Hydro and gas resources. The Fig. 3 shows the Northern Region Power demand of two days i.e. 4th and 5th April, 2020 between the time period of 20 hrs 30mins to 21 hrs.45 mins. It is observed that on 4th April, 2020, power demand is almost constant i.e. around 32000 MW throughout the mentioned time period. But on 5th April, 2020 and at the same time period, there is a huge drop of power demand for a certain period of time. Power falls starts slowly at time of 20hr:30 mins and around at time of 20:55 o'clock, it suddenly falls. It falls from 31000 MW to around 22000 MW. This remains around for 5 mins and then starts increasingly slowly. At the time of around 21:45 o'clock, the power demands returns to its actual position.

The Fig. 4 shows the Western Region Power demand of two days i.e. 4th and 5th April, 2020 between the time period of 20 hrs 30mins to 21 hrs.45 mins. It is observed that on 4th April, 2020, power demand is almost constant i.e. around 33000 MW throughout the mentioned time period. But on 5th April, 2020 and same time period, there is a huge drop of power demand for a certain period of time. Power falls starts slowly at time of 20hr:30 mins and around at time of 20:55 o'clock, it suddenly falls. It falls from 32000 MW to around 24000 MW. This remains around for 5 mins and then starts increasingly slowly. At the time of around 21:45 o'clock, the power demands returns to its actual position.

The Fig. 5 shows the Southern Region Power demand of two days i.e. 4th and 5th April, 2020 between the time period of 20 hrs 30 mins to 21 hrs.45 mins. It is observed that on 4th April, 2020, power demand is almost constant i.e. around 36500 MW throughout the mentioned time period. But on 5th April, 2020 and same time period, there is a huge drop of power demand for a certain period of time. Power falls starts increasing a little at time of 20hr: 30 mins and around at time of 20:55 o'clock, it suddenly falls. It falls from 35000 MW to around 29000 MW. This remains around for 5 mins and then starts increasingly slowly. At the time of around 21:45 o'clock, the power demands returns to its actual position. The Fig. 6 shows the Eastern Region Power demand of two days i.e. 4th and 5th April, 2020 between the time period of 20 hrs 30mins to 21 hrs.45 mins. It is observed that on 4th April, 2020, power demand is almost constant i.e. around 16000 MW throughout the mentioned time period. But on 5th April, 2020 and same time period, there is a huge drop of power demand for a certain period of time. Power falls starts slowly at time of 20hr:30 mins and around at time of 20:50 o'clock, it suddenly falls. It falls from 16000 MW to around 9900 MW. This remains around for 5 mins and then starts increasingly slowly. At the time of around 21:45 o'clock, the power demands returns to its actual position. The Fig. 7 shows the Eastern Region Power demand of two days i.e. 4th and 5th April, 2020 between the time period of 20 hrs 30mins to 21 hrs.45 mins. It is observed that on 4th April, 2020, power demand is almost constant i.e. around 1800 MW throughout the mentioned time period. But on 5th April, 2020 and same time period, there is a huge drop of power demand for a certain period of time. Power falls starts slowly at time of 20hr:30 mins and around at time of 20:55 o'clock, it suddenly falls. It falls from 1600 MW to around 1000 MW. This remains around for 5 mins and then starts increasingly slowly. At the time of around 21:45 o'clock, the power demands returns to its actual position.

CONCLUSION

In this paper, the authors have analyzed the impact on Pan India light out event on Indian electricity grid operation on 5th April 2020 for 9 minutes. Actually POSOCO, the national load dispatch centre estimated this load to be about 12-15 GW and expected it to change in a matter of 2-4 minutes around lights-off and lights-on time. But On 5th April, the actual reduction observed in demand was about 31 GW, almost double the estimated reduction. Still the event was managed in co-ordination with all the stakeholders without any major incident while keeping power system parameters within permissible limits using flexible hydro and gas generation capacity along with advanced grid management actions. Analysis of this successful event management can be considered as future scope of this work.

REFERENCES

1. https://nptel.ac.in/courses/108/106/108106026/
2. https://posoco.in/papers/Reactive%20Power%20&%20Freq_relationship.pdf
3. https://posoco.in/papers/Reactive%20Power%20&%20Freq_relationship.pdf
4. https://www.youtube.com/watch?v=sXmvgDUGiWs&t=1569s
5. https://powermin.nic.in/en/content/power-sector-glance-all-india
6. https://www.youtube.com/watch?v=sXmvgDUGiWs&t=1569s
7. https://posoco.in/download/22-march-2020-demand-comparison/?wpdmdl=27921
8. https://posoco.in/download/22-march-2020-demand-comparison/?wpdmdl=27921
9. https://pmuy.gov.in/
10. https://posoco.in/download/preliminary-report-on-pan-india-light-switch-off-event-on-5th-april-2020/?wpdmdl=28177
11. https://www.prayaspune.org/peg/publications/item/download/709_95c95aa4a9ad64d4f944fc8dcd78000c.html
12. Analysing the Electricity Demand Pattern: http://www.iitk.ac.in/npsc/Papers/NPSC2016/1570293957.pdf

Table IV Region wise details of Expected Load Reduction

Region Wise Details of Load Reduction during Light Switch OFF event on 5th April 2020									
Sl. no.	Region	No of rural household consumers (a)	No of urban household consumers (b)	Load of rural household consumers (mw) (c=50*a)	Load of urban household consumers (mw) (d=100*b)	Reduced load of rural household consumers (mw) (e=c*.80)	Reduced load of rural household consumers (mw) (f=d*.80)	Total reduced demand as reflected at consumer level (mw) (g= e + f)	Total reduced demand as reflected at grid level(mw) (g/0.9)
1	northern regions	42293470	13214064	2115	1321	1692	1057	2749	3054
2	western region	35669904	19020928	1783	1902	1427	1522	2948	3286
3	southern regions	43854642	4668665	2193	467	1754	373	2128	3407
4	eastern region	41183918	4515705	2059	452	1647	361	2009	2168
5	north eastern region	8362568	1689177	418	169	335	135	470	537
6	total	171364502	43108539	8568	4311	6855	3449	10303	12452

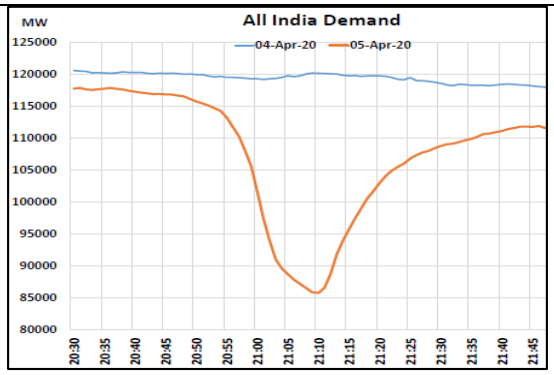

Fig. 1 All India Power demand of two days i.e. 4th and 5th April, 2020.

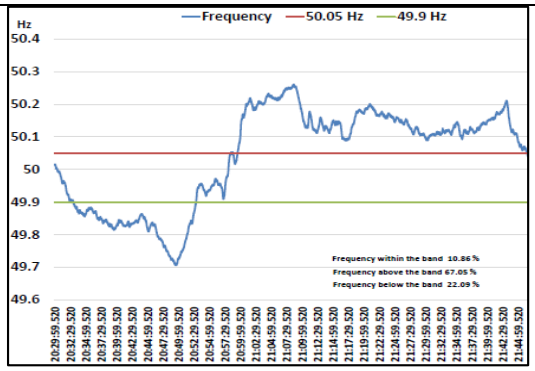

Fig. 2 All India frequency variation.

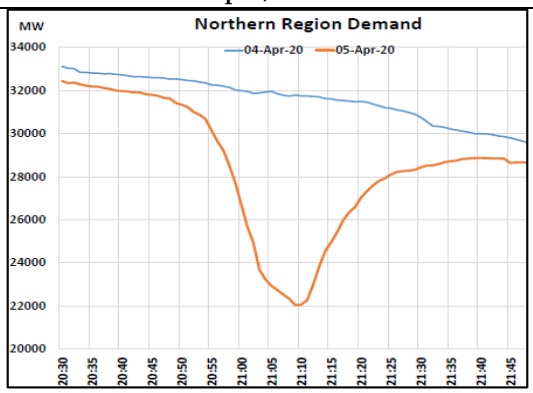

Fig. 3 Northern Region Power demand of two days i.e. 4th and 5th April, 2020.

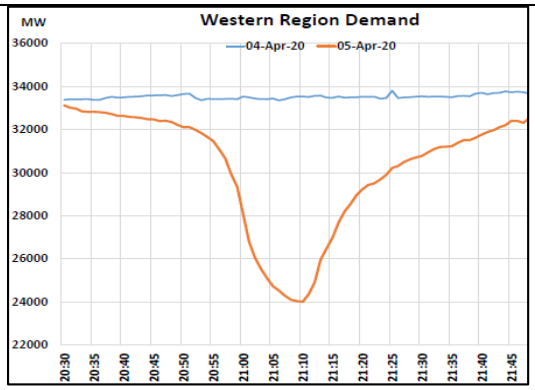

Fig. 4 Western Region Power demand of two days i.e. 4th and 5th April, 2020.

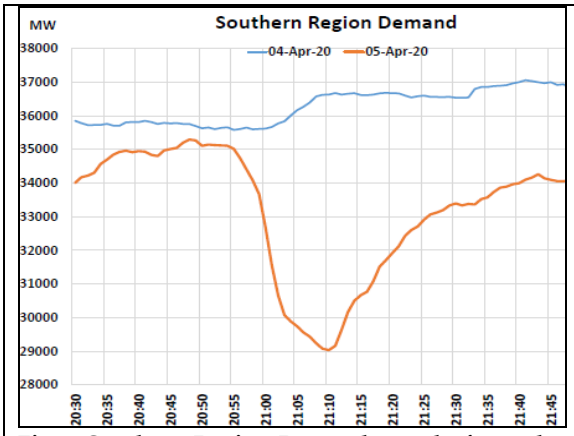

Fig. 5 Southern Region Power demand of two days i.e. 4th and 5th April, 2020.

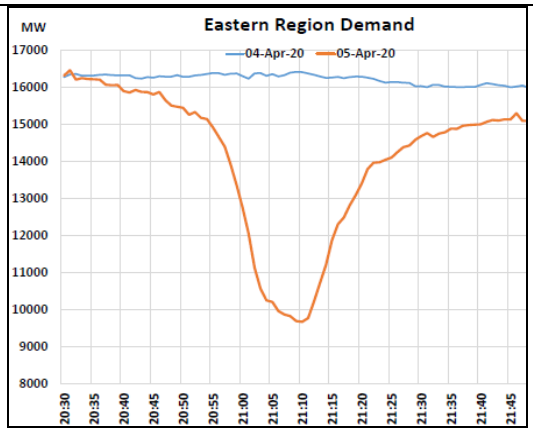

Fig. 6 Eastern Region Power demand of two days i.e. 4th and 5th April, 2020.

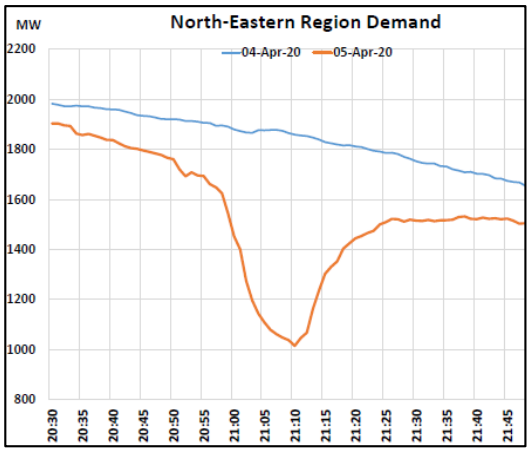

Fig. 7 North- Eastern Region Power demand of two days i.e. 4th and 5th April, 2020.

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RESEARCH ARTICLE

CAN Communication in Automotive Industry

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ABSTRACT

The automobile industry is leading the whole world as it add the economic growth to the society. Anything can be transferred from one place to another place irrespective of the distance. So every day, the new technologies are added to the automotive industries for further increasing of its efficient. By adding new devices, the complexity of the vehicle also increases. The wiring system creates a big problem due to more electronic devices. Each device must communicate each other for proper operation of the vehicle. So, dedicated communication system is required in the vehicle which will manage the vehicle control in a safe manner and makes it simpler. Various communication systems are available where CAN (Controller Area Network) is one the most popular in the industries. It is a high speed communication system and helps to connect more than one electronic system without any computer. With the help of CAN, different Electronics Controller Units (ECUs) can easily communicate with each other. This papers explain about the CAN system and how it worked. In one vehicle, more than one CAN system can be used like high speed CAN and low speed CAN. Based on the priority level, each ECU is categorised to which system it will belong. Other than CAN, other communication system is also used along with CAN. Here, only CAN is explained.

Keywords: Transportation, Automotive Industry, Electronics, Vehicle Communication, CAN Communication.

INTRODUCTION

The transportation system makes the human life easier for transporting everything from one place to another place easily. As it is become the essential for the society, the automobile industry increases there business with various types of transportation vehicles. Every year, the new design and development are coming out by seeing the market

demand. The development in technology makes the automobile industries more effective and efficient performance [1]. Every day, new features are added to the vehicle system which makes the system very complex. To properly manage the whole vehicle, each system must be controlled. Power electronic devices helps to make the system simple and efficient. In the early stage, there was no electronic control. So everything was mechanically controlled. But as the time goes and power semiconductor devices come into market, the automobile industry becomes the major application for the semiconductor devices [2]. There are various devices in the vehicle and each has electronic control unit (ECU). Theses ECUs must communicate each other for the proper control of the vehicle. As the electronic devices increases in the vehicle, the wiring system also becomes more complex and lengthy which increases the cost as well as the chance of faults[3]. To avoid this, the automobile sector uses various communication systems. Those communications are like LIN (Local Interconnect Network), CAN (Controller Area Network), FlexRay, MOST, DC-BUS, J1850, IEBUS, ISO 9141-1/-2, D2B (Domestic Digital Bus), VAN and so on [4]. Based on the requirements and priority, different communication systems are used. In a vehicle, more than one communication systems can be used. Each communication system differs from each other based on their speed, control, priority, number of devices to be communicated etc. [5] Among the various systems, CAN communication is one the most popular system among the above which is adopted by all most all automobile vehicles [6]. It was mainly designed for automobile communications. But due to its simplicity, reliable and high efficient system, its uses are expanded outside the automotive industries such as medical equipment, building automation, agricultural equipment, escalator control, aviation control, navigation system, elevators, various manufacturing industries, robotic, spacecraft, home electronic appliances and so on [7-10]. CAN communication system is developed by Bosch in 1986. In 1993, it is recognised by International Standard ISO 11898. As the no of electronics components increases, the company has also modified the CAN system and high speed CAN come out with more option of connecting electronics devices.

Can Communication System

In a vehicle, various electronic devices are used for different components such as engine controller. Body control unit, door control, airbag unit, brake system, accelerator, door control, suspension, speed sensor, air conditioner, headlight control, indicator, wiper, door mirror, power window control and so on. The Fig. 1 shows the vehicle with different ECUs. ECU is used to control each component. Different ECUs are BMS ECU, ABS ECU, steering control ECU, air bag ECU, suspension ECU etc. To manage all the ECUs, communication is required between the ECUs. Exchange of data and information takes place between each ECU.

The communication may be wired and wireless. But in wireless communication, noise is the major issue. So in vehicle, wired communication is used. The communication is also classified into parallel communication and series communication as show in Fig. 2, respectively. In parallel communication, number of wire is more and each ECU must be connected to other ECUSs. But in serial communication, number of wires is less. Serial communication helps to reduce the complexity, size, reduces the hardware cost and improves the performance in the vehicle. In the early time, the various serial communications were used as as RS-232, RS-422, RS-485, I2C, SPI and microwave. But these have some disadvantage. By considering this, CAN communication protocol is introduced. It is a serial bus communication. The block diagram of an ECU is shown in Fig. 3. It consists of microcontroller, CAN device, ASIC (Application Specific Integrated Chip), timers, signal conditioning, EEPROM, drivers, external I/O. Like this, each device in a vehicle has dedicated ECU which connects each other through CAN bus. Each ECU is termed as node which is connected through CAN bus.

CAN bus consist of two wired system i.e. CAN_H and CAN_L as shown in Fig. 4. It is an asynchronous serial transmission protocol. No clock is used. It is a multi-master based broad casting system. No address is involved in this system while sending the message. It can transfer message with maximum speed of 1Mbps. In this system, anybody can send data at any time when bus is ideal. Message is able to be received by all the nodes. It is an event triggered protocol. Maximum 8 bytes of data in a frame can be transferred. There are two versions of CAN i.e. CAN 2.0 A frame format and CAN 2.0 B frame format. The CAN frame which is less than CAN 2.0 A frame is called standard frame format and which is greater than CAN 2.0 A frame involve both standard and extended frame

format. CAN is based on message based system and prioritization of message is decided by CAN identifier. Smaller the identifier, the higher is the priority of message. Messages like safety critical issue belongs to higher priority. It is liked a plugged-in and plugged-out system. The two wired CAN system is terminated with two resistors valued of 120 Ω to avoid the signal reflection. It is based on wired AND logic

Function of CAN Transceiver

The CAN system consists of CAN controller, CAN transceiver. CAN Controller may be included in the microcontroller or separate devices can be used. It consists of TTL (Transistor-Transistor Logic) logic which operates at 3.3 V or 0V. CAN uses differential voltage to reduce the noise. CAN transceiver converts TTL logic to differential voltage required for CAN bus. CAN message consist of recessive bit and dominant bit. Recessive bit consists of 2.5 V and dominant bit consists of both 3.5 V and 1.5 V and send to CAN_H and CAN_L, respectively as shown in Fig.5.

CONCLUSION

The communication system in automotive industry is explained in this paper. There are various types of communications are there for vehicular application where CAN is one of them and it is the most popular communication. CAN is a serial based communication system developed by Bosch. It reduces the complexity, reduces the size of wiring system, reduces the weight of the wiring systems, and reduces the overall cost. It is a serial based communication and speed is very high. It is a message based protocol communication and multi-master system. Any ECU can send message at any time and everyone can receive the message at the same time. It is a event triggered based communication and based on the priority based, message are sent to the bus. More than one CAN system can be used in a single vehicle. Any number of nodes can be connected to the CAN bus. Details of the CAN bus system is explained in this paper. The CAN message is sent and received by CAN transceiver in each ECU. The differential voltage is used to transmit the message and consists of dominant and recessive bit.

REFERENCES

1. https://injuryprevention.bmj.com/content/8/suppl_4/iv26
2. https://copperhilltech.com/a-brief-introduction-to-controller-area-network/
3. https://www.ni.com/en-in/innovations/white-papers/06/controller-area-network--can--overview.html
4. https://www.csselectronics.com/screen/page/simple-intro-to-can-bus/language/en
5. https://www.allaboutcircuits.com/technical-articles/introduction-to-can-controller-area-network/
6. https://copperhilltech.com/a-brief-introduction-to-controller-area-network/
7. https://www.elprocus.com/controller-area-network-can/
8. https://microcontrollerslab.com/can-communication-protocol/
9. https://www.embien.com/blog/working-automotive-can-protocol/
10. https://en.wikipedia.org/wiki/Vehicular_communication_systems

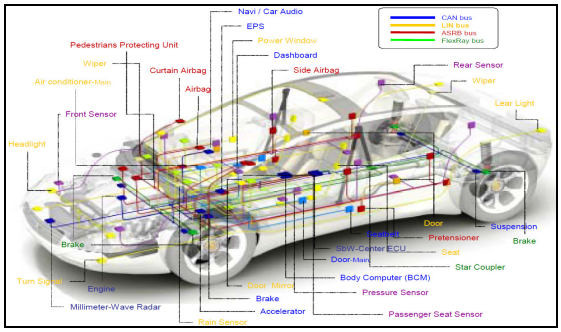

Fig. 1. Different communication system in a vehicle.

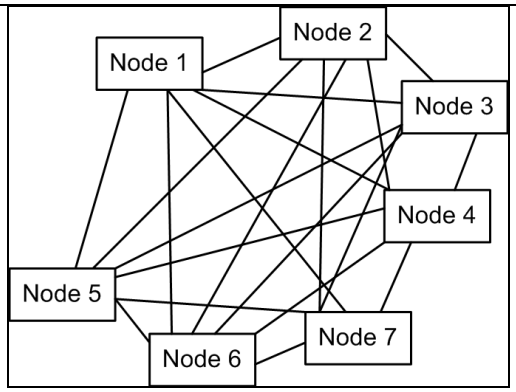

Fig. 2. Example of (a) Parallel communication

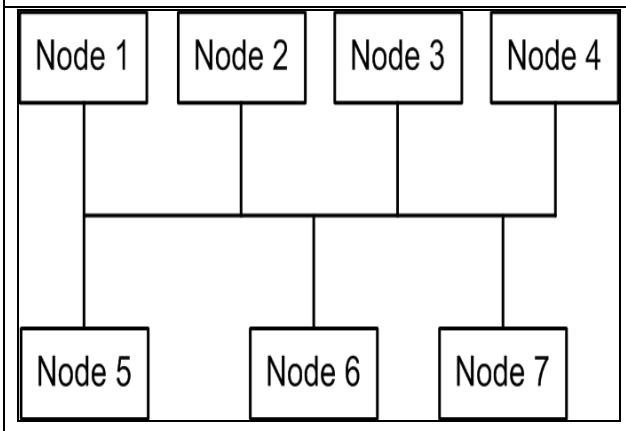

Fig. 2. Example of (b) Serial communication.

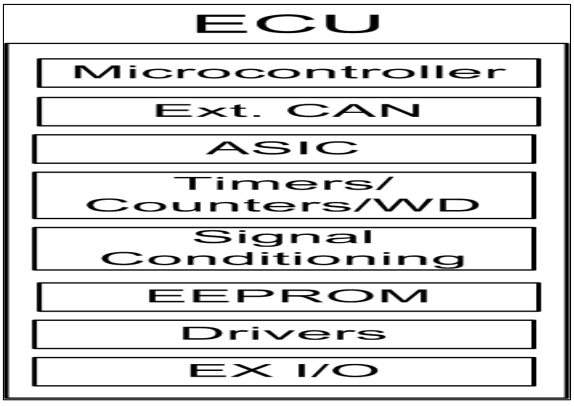

Fig. 3. Block diagram of ECU.

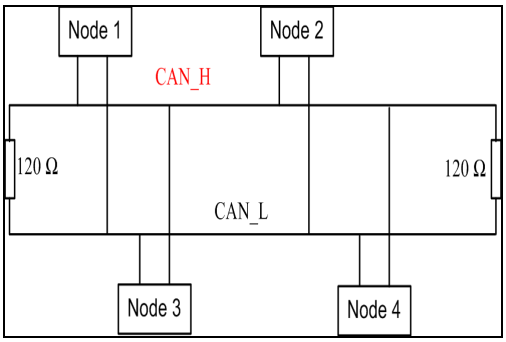

Fig. 4. CAN bus with four nodes

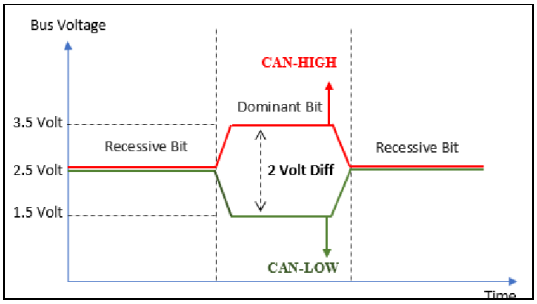

Fig. 5. Voltage level in CAN bus.

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RESEARCH ARTICLE

Role of Women's Organisations in Revitalising Communities: Some Reflections from the Gujarat Earthquake, India

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ABSTRACT

This paper is based on the Gujarat earthquake of 2001 in which there was extensive devastation in Kachchh district in which more than 20,000 lives were lost. It has been almost 2 decades since the disaster and the analysis presented in the paper is a reflection on the role of women's organization in revitalizing the communities. Invariably, women are the most adversely affected, vulnerable to any disaster and they struggle to revitalise their lives and livelihoods typically in a patriarchal setup against a declining resource base. In case of Kachchh, several grassroot organisations have been consistently working with the community women in the villages and have been able to solicit their participation successfully for all the major and specific measures of rehabilitation. Continuation of the livelihood development has been the key to involve women in revitalizing communities. The paper also provides some key lessons learnt from the mutual interaction of women's organisations, with women at the community level during times of disaster.

Keywords: Disaster, Women, Kachchh, Revitalising Communities, Women's Organisations, Gender Sensitivity

INTRODUCTION

More than almost 2 decades have passed since the devastating earthquake struck Gujarat (western State of India) on the 26th January 2001 measuring 7.7 on the Ritcher scale. Kachchh district, the focus of the paper, was worst affected has now a new look today and has been completely rebuilt with the support of the government and 1,800 million dollars, aid received from different parts of the world. The government of Gujarat has been pro-active to rebuild the district by taking it to a new level in terms of infrastructure planning, industries and development. Bhuj town today boasts of a state-of-the art hospital. Today, rebuilding of Kachchh in Gujarat is cited as an exemplary case in major

disaster management forums at the national and international levels. The paper at hand is based on reflections from the 2001 earthquake, particularly the role of women's organisations in revitalizing livelihoods through interventions with the local women and their communities. Lesson learnt can be pointers to revitalizing communities in future disasters in the country and elsewhere.

If one has to go back to 2001, the earthquake in Gujarat had caused extensive damage to life and property. More that 1 million houses were either damaged or destroyed. There were more than 20,000 deaths confirmed by the government. There was massive damage to water supply, electricity and telecommunications, two district hospitals, hundreds of smaller health facilities, thousands of classrooms, office buildings, roads, bridges, dams and reservoirs. Kachchh district is the most affected with maximum number of deaths, injured and loss of property (70% buildings destroyed), infrastructure and other services. The nature of damage caused by the quake was not the same in rural and urban areas. Large number of buildings were completely destroyed in the urban areas, where the number of deaths is higher as compared with the rural areas. In rural areas however, people suffered loss both to housing as well as livelihood (loss of livestock, trees, work sheds, looms, grains etc.). Table 1 provides an overview of the damage in Gujarat and Kachchh in particular.

After the relief period which lasted for three months, rehabilitation and reconstruction programmes were underway in Kachchh for about two years, although the intensity of activities declined. Infrastructure development and new buildings were the order of the day thereafter. Kachchh is the largest district in Gujarat with 938 odd villages and a population of 2,092,371 (Census 2011). Much of the area is arid, that has undergone severe environmental degradation. Kachchh is an area prone to multiple disasters such as droughts, cyclones, floods and earthquakes. Availability of drinking water is a perennial problem in Kachchh villages due to continuous droughts. The population of rural Kachchh comprises 15 different communities (7 Hindu and 8 Muslim groups). There are both mixed and single caste villages found in Kachchh. Each community has a distinct identity in terms of lifestyle (women's clothing, handicrafts and housing). The maps of Gujarat and Kachchh are given in the Figures 1 and 2 respectively.

In urban Kachchh, the four major towns namely Bhuj, Anjar, Bhachau and Rapar were badly hit by the earthquake. In rural Kachchh, 884 villages were affected by the earthquake, of which there was 100% damage in 178 villages and more than 70% damage in 165 villages (Abhiyan/ GSDMA/UNDP, August 2002). The paper is divided into five sections. Observations and analysis pertain to relief, resettlement and rehabilitation programmes in rural areas of the district. After the introduction, the second section deals with the impact of earthquake on the rural communities in general and women in particular. The third section discusses the various organizations engaged in rehabilitation and reconstruction programmes with a critical assessment of gender sensitivity of the same. The fourth section deals with two women's organizations specifically and their role in the process of rehabilitation in rural Kachchh. The last section provides some concluding remarks and lessons learnt. The analysis presented in the paper is based on primary observations during visits to the villages in different parts of Kachchh during the year 2001-2002 and thereafter, detailed discussions with professionals working at the grassroots level with NGOs and other organizations including the government. Primary data pertaining to five villages have been used in looking at the impacts of earthquake on women.

Impact of Earthquake

Apart from loss of life, people in the villages suffered injuries mostly relating to bone fractures, loss of shelter, work sheds (looms), livestock, sources of water and income. It is estimated that among the injured 65% were women (Abhiyan/UNDP, 2001). The reason could be attributed to the fact that when the tremor occurred in the morning, most women were inside their homes. Moreover, when the disaster struck, the *Darbar* (Rajput) and *Syed* (Muslim) women could not rush out of their houses, due to social restrictions. Therefore, in some villages proportionately

more women were injured and lost their lives as compared with men. Besides, women belonging to the scheduled and backward castes such as the *Koli*, *Bharvad* and *Dalits* were particularly hard hit due to their poor economic status (landless and little access to means of income). A survey conducted in 5 villages (N=100) ranked the problems faced by women immediately after the quake during the rehabilitation phase, in the following order: housing (shelter), access to work, health services and schooling for children, access to water resources, livestock, natural resources and other social facilities. Shelter was the first priority for all women for obvious reasons. Lack of access to work was a pre-existing problem that got exacerbated after the quake. The study villages are: Jam Kunaria in Bhuj taluka, Jodhpur Wand and Gagodar in Rapar taluka, Rajansar and Khankoi in Bhachau taluka of Kachchh district.

Women-specific Impacts

The impact of earthquake on women has to be seen in conjunction with drought, which as already mentioned is a perennial feature in Kachchh. Availability of water has implications for women's work. The livelihood strategies practiced by rural households in Kachchh is typical of a drought economy and impose multiple burdens on women. On an average, rural women in Kachchh have a 19 hour work schedule, out of which 3-4 hours is devoted to only fetching water for domestic use. During drought, which happens every other year, embroidery work (traditional craft of women) and government-initiated drought relief work are the main sources of income for women. Upper caste women (Darbar and Syed Muslim) face social restrictions and are dependent on men for livelihood maintenance, which is not the case with lower caste women, although they too have some mobility restrictions. However, economic necessity creates space that allow for negotiation on these norms and other aspects of gender relations (KMVS, 2000). Along with this space, comes the responsibility and burden of household survival. Communities in rural Kachchh are by and large patriarchal in nature, where gender relations are far from egalitarian. Within the framework of gender-based division of labour, women are responsible for provision of household resources (food, fodder and water), care and maintenance of the livestock and agriculture lands. In the wake of the devastating earthquake, women therefore were adversely affected. With regard to the specific impacts, it was observed that wherever women had to support the household single handedly, had been worst affected. Table 2 notes the specific impacts of earthquake on women.

The disaster affected women's income-earning opportunities, particularly sale of handicrafts (embroidery, etc.) with a decline in procurement, as there was disruption in major marketing channels. This was mentioned by 85% of the women surveyed in the 5 earthquake-affected villages. Furthermore, as construction of houses was a priority, women were not in a position to seek wage employment outside. Construction of houses with the support of NGO/government interventions (participatory owner-driven approach) was time-consuming for both women and men, and for which they did not receive any remuneration. Contribution of labour by the owner and his/her family was accepted as part of most housing packages, offered to the people by external agencies. Furthermore, the medical services (free check-ups and distribution of medicines like iron and folic acid tablets, immunization, etc.) that were previously available to women, especially through government and non-governmental channels, were disrupted for a few months during the relief period and partly during the rehabilitation phase and this had a detrimental effect on women's health. About 70% of the women surveyed expressed this fact very clearly, although they included their children's health along with theirs. Shelter construction during the rehabilitation phase was the priority for many NGOs and the government. Other areas such as health and education were neglected. Similarly, schools and *Anganwadis* (childcare centres) in the villages were closed for a long time. Consequently, women's work burden increased considerably as they had to take care of children along with their regular domestic responsibilities, also engage in house construction, and look for alternative wage earning opportunities. Women were also primary responsible for bringing back the normal routine of the household. Similarly, another related aspect of women's health during disasters was availability of adequate nutrition. In Kachchh it was observed that women normally suffered from malnutrition and this had got exacerbated, especially during post-relief phase. During the relief period there was a steady supply of food by different agencies, which lasted a little longer beyond the two months stipulated for relief. Thereafter, people had to fend for themselves. During the transition from relief to rehabilitation phase, there is normally a gap of a few months when both income and food availability declines. The decline and

unavailability of adequate nutrition for women was mentioned by all the women surveyed. As their priority was to reconstruct the damaged houses, women in Kachchh villages were more vulnerable in the transition phase as they were the last ones to get priority in terms of resource allocation at the household level and there was no respite from work (household and community levels).

Post-traumatic stress was a health problem faced by women. Women had a common problem of having to take on the entire responsibility for the household in the event of death of the spouse. They had anxiety during disaster situations and 60% of women expressed that they were suffering from depression and fear. Some of them were not sure about the symptoms and therefore, could not say for certain whether they were affected by stress. In order to make ends meet, women often had to go out in search of employment even in those communities where the mobility of women was restricted. Consequently, there was also the fear and apprehension of losing the goodwill of the community for not abiding by societal norms. The symptoms of trauma were manifested in the form of insomnia, frustration, startle reaction, irritability, anger, guilt, and depression. Kachchh is known to have a high suicide rate among women and this may have increased after the earthquake (although there has been no systematic documentation on this issue). Several NGO personnel working at the grass roots level have corroborated this fact. In the 5 villages surveyed, it was observed that women lived in constant fear of being struck again by an earthquake, as they tend to run out of their houses at the instance of slight tremor.

Despite the wider consequences of a drought-prone economy in rural Kachchh, the impact of disasters such as earthquakes was experienced in the first instance at the household level, where labour is profoundly shaped by gender (E. Enarson, unpublished data). Women's labour which is considered as secondary income for the household played a vital role in sustaining the livelihoods of the households during disaster situations. Worldwide, it was observed that women's daily lives are structured around a complex web of work and responsibilities for family members and the community, for the household economy, to employers, and for the poorest women, to the natural environment which supports them (Enarson, 2001). A study conducted in 141 countries during 1981-2002 in natural disasters and is impact revealed that more women are killed than men especially those belonging to the lower socio-economic strata (Neumayer and Plumper, 2007). The ability of poor women to earn an income every day is crucial for their survival before, during and after disasters (Agarwal, 1990, Jiggins, 1986), and the Kachchh case is no different. Low status and invisibility add to their problems (Doyal, 1995, cited in Daykin & Doyal, 1999). Yet, women manage to contribute to the survival of their families and dependants. What was observed, was that women are actively exploring and using different work strategies in managing livelihoods of their households. Although women's contribution to household survival is indispensable, planners do not pay attention to them while providing institutional support. The next section discusses gender insensitivity in the rehabilitation programmes in Kachchh after the earthquake.

Gender Sensitivity in Rehabilitation Programmes

During 2001, there were 185 agencies working towards rehabilitation programmes in the rural areas of Kachchh. They comprised a mix of state governments, national as well as international NGOs, religious organizations, private/corporate organizations, various partnership organizations and NGO networks. The organizations were engaged in activities related to shelter, health, water/dams, handicraft/livelihood and legal sectors. Most organizations were not gender sensitive, when it came to planning and implementation of various rehabilitation programmes. This was because they assumed that earthquake affects the entire population regardless of gender. Furthermore, the household or the family is the smallest unit of convergent interests wherein all its members share benefits and burdens of existing plans and policies, which of course includes women. The latter is a stereotypical attitude of organizations working in Kachchh as well. It was however observed in the villages of Kachchh that women and children are the most vulnerable due to intra-household inequalities that already existed in the levels of literacy skills, health, nutrition etc. Such disparities tend to get aggravated during times of stress like earthquakes, particularly between the end of relief and beginning of the rehabilitation phase.

There was a distinct lack of gender sensitivity in all the policies and plans that govern rehabilitation and resettlement, as they go by ownership of land or property for compensation and benefits. Since women seldom have ownership rights and further in the absence of any affirmative or progressive clauses to include them, they were automatically left out. This was the situation in general in Kachchh villages during that time. Except for a few organizations, none of them worked with women. Some organizations targeted women for certain activities only in order to attract donor funding. However, such piecemeal efforts failed to make any significant impact on women in rural Kachchh. Two organizations (NGOs) were identified for detailed investigation to understand their contribution towards rehabilitation of rural Kachchh. They were Kachchh Mahila Vikas Sangathan (KMVS) and Self Employed Women's Association (SEWA). Both organizations were Kachchh based and had established their credibility of working with women among the local communities for several years.

Role of Women's Organisations in Rehabilitation Programmes

KMVS and SEWA were the only two Kachchh based organizations working with women in the villages. Kachchh Mahila Vikas Sangathan was a women's organization working in Kachchh for over 30 years. The major objective of the NGO was to enhance the socio-economic and political status of women in Kachchh both at the household and societal level. KMVS believes that in the process women should be empowered and become confident decision making partners in development initiatives at the village, community and regional level. Apart from organizing the collective strength of rural women at the village, block and district level, KMVS aims at building women's capabilities and skills to manage, control, conserve and increase their physical, natural and financial resources. It has been successful in developing local "sangathan" groups into self-governed organizations with development initiatives led by women. These self-governed bodies are expected to control processes aimed at improving the quality of life, especially in the areas of their traditional livelihood (agriculture, craft and livestock rearing), health, access to credit, education and basic facilities (drinking water, fuel, housing etc) and security. KMVS works in Kachchh district alone and is member of NGO network called the 'Kachchh Nav Nirman Abhiyan' or 'Abhiyan', which was very active in the rehabilitation, works in both rural and urban areas of Kachchh. Similarly, Self Employed Women's Association was a member based organization and had established itself as a well-known trade union over a period of about 4 decades. It has over 13, 39, 621 members in the whole country, out of which over 6,99,194 are in Gujarat (SEWA, 2016). Membership of rural women has increased over the years and now they constitute two thirds of the members. Although SEWA started work in Kachchh in 1995, it has been working with women's groups of artisans and savings and credit groups, who constitute the Kachchh Craft Association. In 2018, SEWA started its International Design and Development programme to promote crafts (textile and embroidery) in Kachchh. The attempt by the NGO was to preserve, promote and help market their traditional crafts. SEWA adopts an integrated approach to help women come out of poverty and deprivation. The approach includes organizing for collective strength, bargaining power and representation in committees in the public domain; capital formation through savings and credit, insurance and create assets for women; capacity building for women to compete with the market by providing them access to market infrastructure, information on technology, education, knowledge and relevant skills; social security in terms of health care, child care, shelter and insurance. Both the NGOs have been engaged in the relief and rehabilitation activities in rural Kachchh. Their attempt is not to duplicate their interventions and work in separate villages in the district. Both NGOs work through their respective women's groups at the village level. The rehabilitation programme strategy of both organizations aimed at community based livelihood and shelter reconstruction. The major programmes covered under rehabilitation were:

i) Shelter Reconstruction
ii) Livelihood Security
iii) Social Protection Services

The specific rehabilitation measures included:

i) Housing upgradation and reconstruction of seismic proof houses
ii) Craft as a livelihood security programme
iii) Reviving and regenerating water resources

iv) Health care and nutrition services

Shelter and handicraft related livelihood programmes have been the strength of both the organizations. Strategies adopted by KMVS and SEWA to involve women in rehabilitation works are: involved women in relief distribution at the village level which gave them visibility; ensured that women's participation in the rehabilitation committee meetings at the village level is 50% or more; provided masonry training to women for house construction and building materials (seismic resistant); and ensuring that compensation amount is received jointly by both the women and men at the household level.

For the purpose of detailed discussion, the shelter and livelihood programmes of KMVS and SEWA respectively have been selected.

Shelter

KMVS has adopted a highly gender sensitive and participatory approach in providing housing to the affected households in the village. In all the 13 villages where KMVS is working, there were strong women's groups linked to the NGO activities. They completed 90% of the targeted work, which included 1939 permanent houses in 13 villages. Most of the permanent structures had been designed in a manner which was in tune with the traditional structures (locally called 'bhoonga'). These structures had a round look and had undergone less damage during the earthquake as compared to other houses. KMVS has incorporated certain seismic resistant features to the 'bhoonga' type housing and implemented them in their villages. Both women and men were consulted for adoption of the new structures. KMVS made sure that women's needs were specifically represented. The housing package was such that each household gets two 'bhoongas' (essentially two houses adjacent to each other), which was extremely functional for women as they can cook and store food grains in one and live in the other (smoke-free environment). The idea was to use local materials with slight improvisation for the construction of the 'bhoongas'. KMVS staff informed the author that women were keen to adopt traditional housing interventions, whereas men would generally prefer the typical rectangular houses made of concrete slabs.

In the context of provision of 'bhoonga' type of housing to the beneficiaries, it may be mentioned here that most newly reconstructed houses in Kachchh by a number of organizations have not considered the local designs and have implemented the typical reinforced concrete structures. The reconstructed villages resemble urban colonies completely alienated from the rural surroundings of Kachchh. In the process, the villages have lost their identity. The identity of the NGOs has been strengthened instead. The author has provided a detailed critique of such interventions elsewhere. Therefore, the efforts of KMVS in reconstruction of housing using the local 'bhoonga' designs were laudable.

The most significant feature in providing housing to the beneficiaries at the village level was that the house is registered jointly in the names of both spouses, which is against tradition as women have no property ownership. Initially it was difficult for KMVS to get the women for house registration. However, after much persuasion by a few women leaders (locally referred to as 'ageywans'), both women and men came forward for registration. The other feature was related to building women's capacity in masonry for encouraged them for construction of new housing after the disaster. However, conducting trainings on new technologies and skills was a challenge as women do not want to come out of the villages. KMVS provided training on seismic resistant and other housing techniques to women in different centres locally, where they could have easy access. This was possible with the help of donors and external agencies who were willing to send technicians for the purpose of imparting training to village women. KMVS included harvesting roof rainwater as one of the design features in new housing. The water is collected from the roof and stored in an underground tank. Such an additional feature reduces the drudgery of women having to walk long distances for collecting water. In some of the areas, schools had closed down during and much after the quake. It was observed that the main reason for the closure was not due to damaged school buildings, but lack of proper housing for school teachers which was a problem even before the disaster. As women of the villages were most concerned about education of their children, KMVS took up the responsibility of constructing teachers' housing

quarters as a special project in the vicinity of the villages in one of the most backward areas of the district. It was the government's responsibility to provide housing to the schoolteachers, but KMVS wanted to expedite the construction so as make the local government responsible for the regular functioning of the school and to ensure that teachers live in the same area and are accountable to both the government and the people. KMVS constructed 60 residential quarters in some villages, which would facilitate 42 villages of the area for 60 schools (Abhiyan/GSDMA/UNDP, 2002). Such efforts had the potential to improve the attitudes of people towards education, particularly for the girl child.

Livelihood Restoration through Handicrafts

Kachchh is an area famous for its handicrafts especially embroidery work by women. There are 8 different communities living in the district and each one has a distinct embroidery style. NGOs such as KMVS, SEWA, Kalarakhsha and Shrujan were engaged in promoting handicrafts made by village women. Marketing the products is a challenge for the organizations post-quake.

SEWA worked with 12,000 women artisans in 135 quake affected villages during 2001. Each artisan had been provided with a craft kit/bag with raw materials for a week's work. Every week, the spearhead team from SEWA collected the finished goods and made the payment of RS 40 per day (2001 minimum wages) at their homes. Women were paid in both cash and kind (food grains or clothes). SEWA had also planned worksheds for the artisans in some villages. In order to promote handicrafts, SEWA organized several exhibitions for sale of products in different parts of Gujarat and outside. Both SEWA and KMVS mobilised self-help groups (SHGs) of women for the purpose of savings and credit. These SHGs had the potential to act as collectives for different economic activities. KMVS and SEWA had organized 8603 and 4496 women through 209 and 277 SHGs in 147 and 87 villages of Kachchh respectively (Abhiyan/GSDMA/UNDP 2002).

Here is what some women artisans had to say with respect to SEWA's interventions:

Jamunaben an artisan from Dhokawada village says – *"Craft work not only gives us work and employment. It gives us dignity. It helps us live a dignified and decent life amidst such a disaster".*

Others join her saying – *"Yes, we do not have to borrow for our daily necessities. This gives us and our families tremendous sense of security and self- respect. Otherwise we would be vulnerable and at the mercy of moneylenders".*
Manchabaa says – *"By giving us immediate work, you have not only provided relief to us but also dignity and recognition. Our skill has now been recognized. How long can we survive on relief supplies? It is work that helps us survive and rebuild our lives".*

Organisations such as SEWA restored the confidence of women who had been under tremendous mental and physical pressure after the quake. It is women's income through handicraft work that contributes to the survival of households, where all assets were damaged or completely destroyed. Invariably, households were waiting for the 'compensation money' to be given by the government and alternative means of income for the male members. Some of the other programmes implemented by KMVS and SEWA played a significant role in revitalizing the quake-affected communities in Kachchh. They are discussed in the ensuing sections.

Fodder Security System

SEWA was engaged in provision of fodder to 350 families to support 2204 cattle heads. The process involved placing order and procurement of fodder, planning the delivery mechanism, organization of the distribution process, deal with and negotiate with aggressive men, quality checking, assess the needs and keep records for the government. Active women members of the collectives efficiently performed all the above activities.

Restoration and Construction of Water Sources

Water scarcity as mentioned in Kachchh is a perennial problem. The destruction of irrigation structures, small dams and drinking water tanks and pipes had further exacerbated the problem especially for women. Both the organizations were working on promoting, revival and construction of water harvesting structures. Small dams and other water harvesting structures had been repaired before the onset of monsoon. KMVS was particularly interested in reviving the traditional water sources such as ponds and 'virdas' (shallow ponds). As already mentioned under the shelter programme, design features related to rainwater harvesting in housing had been introduced and proved to be a success among women. They had received training by NGOs to maintain the water infrastructure.

Drought proofing programme initiated by Abhiyan (network of 29 NGOs) with the support of the Prime Minister's Relief fund, was the major activity that aimed at strengthening the existing water resource structures, enable dry land farmers to grow at least one crop, increase productivity of grasslands, arrest migration from villages and bring greater community control (strong women focus) in drought relief work. KMVS was one of the member organizations pro-actively engaged in the drought proofing programme. The major activities in the drought proofing programme were: upgradation of traditional water structures, construction of new ponds, construction of percolation dams, well recharging, farmland bunding and grassland restoration and development.

Support Services (Childcare, Education, Insurance, Savings and Credit)

SEWA and KMVS emphasized on starting the childcare centers and primary schools in the villages. It required lobbying with the government to shift priority to social services and not focus only on housing. Government and UNICEF responded to the demands of the women's organizations positively - insurance and credit services were extended to women to take care of their income needs. Similarly, health services were also being revived gradually for women.

Dialogue and Interaction with the Communities

Through their respective mediums (newsletter, radio and satellite programmes) both SEWA and KMVS had conducted regular interactive sessions on the rehabilitation plan, government's different shelter packages, policy, the significance of seismic proof construction etc. Such interactions help women to understand the significance of organizing and to overcome stress and trauma, the relevance of micro-finance and SHGs, insurance and childcare services in protecting and securing their lives and their livelihoods during times of disaster. Discussions with personnel (professionals as well as village level workers) of both organizations brought out clearly that during the relief phase, women's groups were less driven by caste and religious sentiments. Women were sincere and concerned about the welfare of the entire community. Although the approach of both KMVS and SEWA were to work through women's groups in the villages, but it had implications for the entire community. KMVS staff mentioned that they had been successful in mobilizing women to come forward and participate in implementation of programmes and various trainings related to rehabilitation. But their experience had been that wherever women participated, they put in their best, attended meetings on time, maintained transparency in accounts and other records. Women's consistent participation in the rehabilitation programmes had strongly facilitated both the organizations in implementation at the village level efficiently.

CONCLUDING REMARKS AND LESSONS LEARNT

This paper is based on observations and data gathered during the years 2001-2002. The lessons learnt from role of women's organizations in revitalizing the communities have its relevance today as disasters are a regular feature in India. There is a differential and adverse impact of earthquake on women in terms of casualty, injury, trauma, insecurity, income earning and household responsibility. Women's indisposition affects the functioning of the households and therefore their well-being is of prime concern especially during times of stress. Women's participation in relief and rehabilitation can better address not only, women's needs but also, the needs of the community in terms of prioritizing needs, implementing programmes and monitoring progress. It was observed from the foregoing sections that women's organizations such as KMVS and SEWA are in a better position to address

the communities' needs compared with other organizations in terms of addressing equity and other concerns which are invariably neglected. Consistency in women's participation has facilitated the smooth implementation of the rehabilitation programmes. In general, there is a need to factor in gender sensitivity in the post disaster relief and rehabilitation programmes especially looking at the needs of women. It is necessary to include women's and men's voices, needs and expertise equally in disaster risk reduction (DRR), and recovery policy and programming (UNDP, 2010). Attention needs to be paid to women's capacity to manage risks, with a view to minimize their vulnerability and enhancing their opportunities for development. What is generally observed is that women's vulnerability in disaster situations is highlighted, but their potential roles in DRR have often been overlooked (IUCN, 2009).

Lessons learnt

1. Women's groups should be involved in the relief programmes at the village level as they have proved to be sincere and transparent in the task.
2. Women's sense of functional space in the house is important to consider and therefore their participation in reconstruction should be solicited, especially when traditional features of housing are retained.
3. Additional housing features for disaster resilience and water harvesting will not only, help women, but also their families in the long run.
4. The transition between relief and rehabilitation is most critical for women as they would need special attention in terms of food, medicine and child care.
5. Training women in masonary and building water infrastructure like roof rain water harvesting will not only, ensure that they are empowered but also, break gender barriers and change gender relations.
6. Promoting women SHGs (self-help groups) in capacity building for livelihood development and insurance is important in disaster situations.

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REFERENCES

1. Abhiyan and UNDP (2001), *Coming Together*, Bhuj (Kachchh).
2. Abhiyan/GSDMA/UNDP (2002), *Coming Together*, Bhuj (Kachchh).
3. Agarwal, B. (1990), "Social Security and the Family: Coping with Seasonality and Calamity in Rural Indi". *Journal of Peasant Studies 17* (3), 341-412.
4. Daykin, N. and Doyal, L. Eds. (1999), *Health and Work: Critical Perspectives*. Basingstoke: Macmillan Press Ltd & New York: St. Martin's Press.
5. Enarson, E. (2001), *Promoting social justice in disaster reconstruction: guidelines for gender-sensitive and community-based planning.* Ahmedabad: Disaster Mitigation Institute.
6. Government of India. (2011), District Census Handbook, Directorate of Census Operations, Gujarat.
7. IUCN (2009), How Natural Disasters affect Women (https://www.iucn.org/content/how-natural-disasters-affect-women)
8. Jiggins, J. (1986), "Women and Seasonality: Coping with Crisis and Calamity", *IDS Bulletin*, 17 (1).
9. KMVS (2000), *Flying with the Crane: Recapturing KMVS's Ten Year Journey*, Bhuj.
10. SEWA (2016), http://www.sewa.org/About_Us_Structure.asp
11. SEWA (2001), *Rehabilitation Package Notes*, Ahmedabad.
12. Neumayer, E. and Plumper, T (2007), "The Gendered Nature of Natural Disasters: The Impact of Catastrophic Events on Gender Gap in Life Expectancy 1981-2002", *Annals of Association of American Geography*, 97(3), 551-566.

13. United Nations, GSDMA and GOI (May 2001), *Conference Proceedings of Sustainable Recovery and Vulnerability Reduction*, Ahmedabad.
14. United Nations Development Programme (2010), *Gender and Disasters*, Bureau of Crisis Prevention and Recovery

Table 1: Devastation due to Earthquake at a Glance

Devastation	Number
No. of districts affected in Gujarat*	21
No. of talukas affected	182
No. of villages	7,904
Total number of human deaths	18,253
Number of deaths in Kachchh	16,681
Total number of persons injured	1,66,836
Total number of persons injured in Kachchh	1,36,048
Number of 'Pucca' houses destroyed	1,59,960
Number of 'Pucca' houses damaged	3,99,346
Number of mud houses destroyed	1,48,339
Number of mud houses damaged	2,95,061
Number of huts destroyed	13,889
Number of huts damaged	31,395

Source: Government of Gujarat, February, 2001 * Gujarat State has 25 district

Table 2: Specific Impacts of Earthquake on Women (N=100)

Impacts	Yes (%)	No (%)	Not sure (%)
Income earning through sale of handicrafts	85	5	10
Disruption of existing medical services	70	7	23
Inadequate nutrition	65	15	20
Post-quake trauma	60	26	14
Insecurity	64	14	22

Source: Primary survey in 5 villages of Kachchh, 2001

Note: The questions relating to the responses in the above table were asked to women alone, without the involvement of men. It was observed that the response 'not sure' may also imply that they were unable to comprehend the question or they may not have been affected directly.

Figure 1: Geographical map representing Gujarat

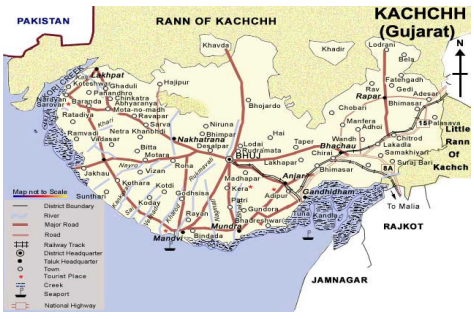

Figure 2: Geographical map representing Kachchh of Gujarat

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RESEARCH ARTICLE

Social Dimensions of Post-quake Programmes in Kachchh, Gujarat (India): Disaster Management Lessons

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ABSTRACT

This article focuses on the social dimensions of post-quake rehabilitation programmes in Kachchh district of Gujarat state (earthquake of Jan 2001) in India. Several rehabilitation and reconstruction packages were undertaken by the state, NGOs, and other organizations, either independently or on a partnership basis. The focus is on rural Kachchh and the different shelter programmes. rehabilitation and resettlement programmes of a large magnitude, are bound to be ridden with problems. The issues covered are loss of village identity, caste/community politics, NGO dynamics in rehabilitation programmes, lack of gender sensitivity in the programmes and dependency syndrome with respect to the affected population. Some disaster management lessons have been derived keeping in mind the needs of the rural population, class and particularly with respect to the role of the government and the NGOs.

Keywords: Kachchh, Gujarat, Earthquake, Rehabilitation, Social Dimensions, NGOs, Disaster Management

INTRODUCTION

More than two decades have passed since the great earthquake hit Gujarat state in India in January 2001. Kachchh was the most affected district in the state. Immediately after the earthquake the government as well as several external agencies undertook rescue and relief works. Rescue operations came to a halt after a fortnight, whereas relief programmes continued till the end of March 2001. There was a gap of 2-3 months before rehabilitation programmes were actually launched as they had to be planned in detail and further entailed huge funding. In Kachchh, rehabilitation programmes were initiated in full swing in June 2001. The magnitude of devastation was such that it was not possible for the government alone to undertake rehabilitation and reconstruction works in the affected areas. The focus of this paper is on quake-affected villages of Kachchh only. After the introduction, the

second section delves into the social dimensions of rehabilitation programmes. Shelter programmes have been taken up as an example for detailed discussion while looking into the social dimensions of the rehabilitation programmes. This is followed by some concluding remarks and lessons. The analysis presented in the paper is relevant in the context of disasters rehabilitation, reconstruction and provision of housing is a priority in post-quake situations anywhere in the country.

In Kachchh, the rehabilitation and reconstruction was typically provided in the form of compensation packages for loss of kin, injuries to the human body, damage to housing and loss of livelihood sources both by the government and non-governmental sources (NGOs, national and international donors, private organizations, religious organizations and various networks). There were several other programmes relating to infrastructure and social facilities for development of the area as a whole. As of September 2002, there were 185 agencies including 4 state governments working in different sectors of rehabilitation in rural Kachchh. The different sectors of rehabilitation are: Shelter, Water/Dams, Handicraft/Livelihood, Education and Health (Abhiyan/GSDMA/UNDP, 2002). Shelter was the most visible programme of the rehabilitation process in terms of investment and number of housing units constructed. It was a priority for the people affected in the earthquake. What was further seen is that several organizations found it easier to mobilize huge amount of funds for shelter programmes as it involved tangible outputs.

The example of shelter has been taken up in the paper for illustration of a rehabilitation programme. There were three kinds of approaches to provision of shelter. They are as follows:

a) Self construction by the villagers with the compensation money received from the government (amounts varied according to the intensity of damage to the houses)
b) Government-NGO partnership (50-50 basis)
c) Reconstruction done by the NGOs alone

Out of the total of 89 NGOs working in the shelter programme, 68 were part of the public-private (Govt-NGO) partnership, while 21 had been working independently. Similarly, were many villages where no organization had been able to work for several reasons and people had decided to go for self-reconstruction of houses, with the help of compensation money received from the government. The NGOs working independently may operate alone or in partnership with other organizations (a network of NGOs or with private/corporate sector). At the end of August 2002, a total of 140 villages had been reconstructed with a total of 13,930 houses by 53 NGOs (Abhiyan/GSDMA/UNDP, 2002). According to the 2002 report, the number of temporary shelter units provided by NGOs was 81,197 in 877 villages. The requirement for permanent shelter is 1,11,786 units. The plan was to construct 48,379 houses by NGOs.

Rehabilitation and reconstruction programmes continued for two years in rural Kachchh. Thereafter the attention shifted to the urban towns that needed institutional support for reconstruction.

Social Dimensions

The analysis presented pertains to observations made during the process of implementation of the rehabilitation programmes and after the completion of the activities in affected villages only. In rural Kachchh, 884 villages were affected by the earthquake, of which there was 100% damage in 178 villages and than 70% damage in 165 villages (Abhiyan/GSDMA/UNDP, 2002). It may be noted at this point that the social dimensions discussed are not similar to cases where rehabilitation has occurred due to evacuations as a consequence of dam construction or multi-purpose projects. In case of the Kachchh earthquake, response in terms of rehabilitation and support had to be immediate and on an emergency basis. Newspaper reports mentioned that the recovery and reconstruction in Kachchh had been faster as compared with the rest of the country where calamities such as cyclones, floods and typhoons keep occurring every year in the country. However, in spite of the best efforts by the government and various agencies, there were several lapses in the approaches, designing and implementation of the rehabilitation programmes, which had significant social implications for the rural population.

Although there were some evaluation studies of the different rehabilitation interventions but the social dimensions of rehabilitation and reconstruction programmes were not documented systematically, although they did surface at times in discussions with NGOs and professionals working in the area. The social dimensions (latent or manifest) of rehabilitation discussed in the paper are based on observations made with respect to the approaches and the process of implementation of different interventions as well as after the programme had been completed. Rehabilitation works started in June 2001 and continued for 2-3 years although many shelter programmes were completed within one year. The issues discussed in the ensuing sections are based on observations at the micro-level.

Loss of Village Identity

After almost three years of continuation of rehabilitation and reconstruction programmes, involving several NGOs and other organizations including 4 state governments engaged in building houses, one is struck by the huge hoardings and arches (both temporary and permanent) carrying the names of the organization, donors, number of houses and other infrastructure provided. The hoardings were meant to display the achievements of the organization. These organizations had intervened both in terms of in-situ rehabilitation as well as relocating parts or entire villages. Most of them were not Kachchh based, working in affected villages for a short term basis. The investments made by the organizations for the shelter programmes were also mentioned on the boards/hoardings in some cases. The name of the village was invariably changed or had the term "New or Navi" prefixed to the old name, meaning that it had been newly reconstructed. The new name of the village may be taken after the leader of that organization engaged in the shelter programme. The old name is written is small letters and at times mostly invisible. The traditional housing structures had been completely replaced by new ones (modern seismic resistant designs developed by the organization with technical assistance from renowned institutions). The new structures had given an identity to the organization engaged in the reconstruction works. From a distance, one is able to make out the identity of the organization. The newly constructed villages look like independent urban colonies and not like villages anymore. The new settlement structure of the village does not blend with the habitat of rural Kachchh. They were typically regimental structures with no regard for cultural space of the communities. After occupation, people made extensions of wooden twigs and dried leaves to accommodate their livestock, which was not planned in advance by any of the intervening organisations. Bathrooms and toilets provided by the organizations had been invariably converted into storage rooms for hay and firewood. People found it difficult to adjust to the new type of concrete structures. The older people in the villages were not happy with the way the NGOs and other organizations have overshadowed their identity. It should be noted that the identity of the Kachchhi people comes from their clothing, housing and lifestyle. What was observed is that the NGO space has ascended on the life space of the people of the rural communities, thereby diluting their identity. One NGO professional remarked,
"Villagers are unable to give up their rural lifestyle and identify themselves with the urban population. That is the reason why villagers feel out of place in such new surroundings".

In contrast there were a few Kachchh-based NGOs like the Abhiyan network of NGOs and others who were sensitive to the traditional lifestyle of the people and thereby encouraged them to adopt housing structures that were closer to the ones they owned. One such example is the traditional housing structure called *Bhoonga* housing, which is round shaped and functional for women, because a rural household in Kachchh would normally possess 2 such structures, one for cooking and storage and, the other for living[1]. As part of the shelter package, the NGOs upgraded the *Bhoonga* with additional features for seismic resistance and offered to the villagers for adoption. However, only about 30 villages adopted *Bhoonga* type of housing in Kachchh. The rest adopted the typical reinforced cement concrete structures (one or two room units), as they resembled urban housing and were considered superior to the traditional type of housing.

Social Divisions and Caste/Community Politics

Rural Kachchh is inhabited by 7 Hindu and 8 Muslim groups with several sub-divisions. Caste and religious differences were strongly represented in villages, although no major communal conflicts have occurred in Kachchh district unlike other parts of Gujarat. There were several faith-based and other organizations working in Kachchh

towards various rehabilitation programmes. Some of them tend to work with certain castes or ethnic groups, in terms of providing housing and other facilities including cash donations. The motive of such organizations was to help those people (followers) who show allegiance to them. There were cases where faith-based organizations had been instrumental in relocating some groups out of the original village, either to a close-by location or to an entirely new area. They may even provide new housing to the groups in the same village. Such sectional assistance to specific communities had created latent tensions in the villages. Those who had not got preferential treatment or had been left out expressed their anger about the same. NGO functionaries feel that such latent tension may lead to conflict in the future, on caste and communal lines as existing social divisions get sharpened over time.

Whereas, there are some pro-people organizations that had planned to provide housing of the same type to the entire village regardless of their caste and religious affiliations. Such initiatives had often also been met with resistance from the richer castes (Patels) who would decline to accept one or two room units. Their argument typically would be that the rich and the poor cannot be treated alike. Whereas, the lower castes and tribals (Harijans, Rabaris and Kolis) were willing to accept whatever came their way. There had been many cases where due to lack of single consensus among the people in the *gram sabha* (village council), the organizations would get discouraged and abandon the affected village.

The other side of caste politics related to restricting entry of NGOs to the villages for reconstruction by the richer/higher castes. It is a well-established fact that the earthquake had affected the poorer sections of the society much more than the rich (land owning Patels) and upper castes. In many cases, the latter did not want NGOs to facilitate reconstruction programmes in the villages, as it would empower the lower castes (poorer groups) and subsequently threaten their hegemony and dominance. Some of the richer castes went to the extent of bribing the NGOs not to enter their villages (based on personal communication with NGOs in Bhachau, Feb 2001).

Another aspect of how social divisions within the community get perpetuated through external agencies is the relocation packages offered by the government in the form of titles for housing purposes. The government of Gujarat announced certain entitlement norms for village relocation (although only 16 percent of the villages opted for either partial or complete relocation). They are: a landless agriculture labour was entitled to 100 sq m of plot area and 30 sq m for construction; a marginal farmer up to 1 hectare landlholding was entitled to 150 sq m of plot area and 40 sq m for construction; a small farmer with 1-4 hectares of land was entitled to 250 sq m of plot area and 40 sq m for construction; and a farmer with more than 4 hectares of land was entitled to 400 sq m of plot area and 50 sq m for construction (Gujarat State Disaster Management Authority, 2001). There was a clear discrimination in provision of land for constructing new houses by landholding size and class and not by the extent of damage to the houses.

NGO Dynamics in Rehabilitation

Several NGOs (national and international) were engaged in rehabilitation programmes in different parts of Kachchh. Although there was a regulation on paper, where the NGO had to obtain permission from the district administration to intervene in a particular village, it was observed that there would be more than one NGO in the village working in the same programme e.g housing or livelihood. Each wanted to establish their credibility in undertaking rehabilitation programmes in Kachchh and therefore would want to ensure that they have the support of the community. They would resort to use of several methods to obtain the support of the people like a particular section of the village or some groups within the community in order to capture their area of operation. They would engage in handing out cash doles, food, drink (alcohol) and in merry making. Such NGOs were mostly from outside the Kachchh district and were based in the earthquake-affected area for short periods. It is obvious that their credibility in terms of achievements and popularity is linked with the sustenance of the organization for future donor funding.

It is common to find NGO leaders addressing a crowd of villagers. An example can be cited here. It happened in Rajansar village of Bhachau taluka (sub-division of Kachchh district). A NGO leader was addressing a group of poor villagers belonging to one particular community. His address was as follows:

"All of you are poor people. Nobody cares for you. The rich and the powerful have cornered all the benefits. The government is useless and cannot do anything for you. It is blind to the needs of the poor. It is not sensitive to the needs of the people and this is reflected in the policies, which are anti-poor. The poor are being cheated and given housing which costs much less than what the rich get. We want to help you. All those of you who want help, may mention their problems and names in the list that I am circulating…." (taken from Nitin P. Agarwal's field notes, Jan 2001) [2].

Based on personal discussions with professionals working with Abhiyan[3] and GSDMA, the author was informed that such instances (mentioned above) were very common, where NGOs address villagers, maligning the work of the government and other NGOs. As a result, villagers were confused as to whom to trust and which programme to accept. NGOs have their own agenda and at times are not concerned with the true welfare of the people. It is common to find a number of hoardings publicising the works of different NGOs in one village. Such villages are generally located on transportation routes that have easy access from the main urban centers. There is a tendency among NGOs to select those villages that are socially homogeneous with minimal caste politics. In addition, they would want to intervene in such a manner so that they could complete construction work in short periods and leave early (e.g construct 400 houses and leave in 2-3 months' time). The contractor would be interested in such an approach as it brings good profits. An interesting example can be cited here of relocation of village *Dudhai* by the former Chief Minister of Delhi under the aegis of *Swabhiman Trust*. The village was renamed as Indraprastha and was the first village to be reconstructed in 3 months' time. The Prime Minister of India inaugurated the village on June 4, 2001. It contained 800 one room units of cement concrete blocks. It was reported that 200 Patel families refused to move into the new houses, which they felt was below their dignity (Mahadevia, 2001). The new village had all the facilities, such as, their own power supply, water supply, school and health centers. Yet people do not want to leave their traditional lands and homes. Most of the occupants of the village belong to lower castes and found it convenient to relocate because of their already disadvantaged position in the village.

Another example can be cited here regarding the different housing packages of the NGOs. The packages are as follows: one which costs Rs 45,000 (approximately US $ 1000 by 2001 rates) with owner's contributory labour, another package for Rs 100,000 (approximately US $ 2,000 by 2001 rates) with no contributory labour and yet another for Rs 200,000 (US $ 4,000 by 2001 rates) with added incentives. With an influx of NGOs offering different housing packages, confusion among local people is inevitable and can potentially hamper the progress of rehabilitation. The poor villager is inundated with offers, which she/he has never experienced in their life-time. Additionally, in such situations, it is difficult for villagers to arrive at a consensus and this can lead to further divisions among the village community, where several factions spring up aligning themselves with different NGOs. In one such village in Rapar taluka (sub-division of Kachchh district), an NGO had come to an agreement with the people regarding the assistance including house design and accordingly unloaded raw materials in the village. After a week or so, the villagers declined the offer and wanted the materials to be removed from the village. No amount of persuasion mattered and the raw materials had to be removed and further the organization had to pay rent for the space in the village. The reason for such an attitude by the people is obvious. They were offered a better package by some other organization.

It may be noted, that NGOs in Kachchh have been able to operate after the earthquake because it was not possible for the government to provide rehabilitation support to all the affected villages. As the number of NGOs working in the area were too many, there was competition among them to establish their credibility, which was eventually linked to their future funding and sustenance. Instances of animosity and in-fighting among NGOs leads to mistrust with the people. People take advantage of the situation and add fuel to the fire. In such situations, local communities inadvertently become dependent on external agencies for support, which can potentially prove harmful for the future development of rural Kachchh.

Lack of Gender Perspective in Rehabilitation Programmes

In the entire rehabilitation operation, it was observed that except for 4 organisations, none were inclined to include gender in their agenda. This was because it was commonly assumed that earthquake affects the entire population regardless of gender. And further, the household or the family is the smallest unit of common interests wherein all the members shared benefits of existing policies, which of course includes women. However, it was observed that women and children are the most vulnerable due to intra-household inequalities that already exist in the levels of literacy skills, health, nutrition etc. Such disparities tend to get aggravated during times of stress such as earthquake, particularly between the end of relief and beginning of the rehabilitation phase. It was observed that women could not move out of their villages during the reconstruction of housing, as they felt insecure to leave their belongings in the open. As a result, they lost out on wage work, available outside the village.

Similarly, there is a lack of gender sensitivity in all the policies and plans that govern rehabilitation and reconstruction as they go by ownership of land or property to be eligible for the same. Since women seldom have ownership rights over property and with no affirmative action to back them, they were automatically left out. In Kachchh villages too the situation was no different. However, there were NGOs like the Kachchh Mahila Vikas Sangathan (KMVS) and the Self Employed Women's Association (SEWA) who work only with women for all post-quake programmes. Such NGOs ensured that in their housing programmes, women not only, select the design but also, obtain joint-ownership of the housing unit after completion. They also ensured that the housing design is conducive to the traditional lifestyle of women (e.g *Bhoonga* housing) and wherever possible provided means for roof rain-water harvesting and storage in underground tanks close to the house in order to facilitate collection of water. None of the other housing packages have thought of this need of women. Besides KMVS and SEWA could secure the support of local communities as they have engaged in livelihood provision through women's collectives.

Some organizations wanted to show that they were gender sensitive and would encourage women to speak up in the gram sabha (village council). The men-folk would sense that there is some gain in the form of cash or incentives and would encourage their women-folk to participate in public meetings. But such gestures had minimal impact. However, many organizations felt that their approach left out women and the programme could have been better implemented in a much better manner had they participated in the planning phase (personal communication with NGO professionals and several donor agencies working in Kachchh, December 2002).

Dependency Syndrome

Rural communities in Kachchh were known for their resilience and hard work. They would not prefer to ordinarily accept doles from external agencies during emergency times. This attitude was reflected during the relief phase when food, clothes and other items were being distributed. People would refuse to accept more than what they needed and after the initial hardship were prepared to work for their living and not depend on relief camps. It was reported in various Newspapers, how the Kachchhi villagers would refuse to accept relief and always took pride in their tradition of being perfect hosts. However, today with so many organizations intervening for different programmes and with huge amount of funds flowing in, villagers had become dependent on outside agencies. They were not willing to work as long as there was support from outside. Discussions with various established NGOs (professionals and workers at the grassroots level) reiterates the fact that villagers had become too much dependent on outside agencies for support. All activities in the villages seemed to be donor driven. Such dependency poses a danger to the future of the people and could hamper indigenous development.

The dependency syndrome created by the NGOs and other external agencies was a manifestation of too many organizations attempting to help the rural population of Kachchh. Influx of NGOs for rehabilitation works and their concentration in those villages, which had easy access in terms of transportation, had led to a situation where the supply is much more than the demand. Consequently, there was competition and conflict among different NGOs. This had in a way diluted the credibility of Kachchh-based organizations. Kachchh-based NGOs felt that the greatest challenge for them was to get rid of the dependency of the local populations for external support.

CONCLUDING REMARKS AND SOME LESSON

The foregoing sections provides an account of the social dimensions of rehabilitation after the Gujarat earthquake of 2001. Rehabilitation and reconstruction programmes in Kachchh after the earthquake was bound to be ridden with problems. It was observed that the rehabilitation policies and programmes of the government had been favourable to the rich than the poor and this had accentuated the existing inequalities. Similarly, the programmes of the NGOs focusing solely on specific religious communities or deprived sections of the society had generated resentment amongst the privileged sections of the society and it had exacerbated the existing social differences and tensions. Women's concerns had largely remained neglected in the rehabilitation programmes. Some villages had lost their old identity due to partial or complete relocation. Unhealthy competition among NGOs and overcrowding in rehabilitation works created problems for both the NGO sector itself as well as the efficacy of the rehabilitation works.

Lessons

Keeping in view the immediate needs of the rural population in Kachchh post-quake and the fact that certain interventions had potential to create social tensions, some lessons were derived followed by suggestions relating to the role of government and the NGOs. Such disaster management lessons are applicable to any post-quake situation, where external agencies are engaged in relief and rehabilitation including reconstruction. They are as follows:

1. Government could play a more pro-active role in the rehabilitation process. Although the partnership approach to housing is in place, government's role in support and monitoring progress was minimal. At times people have objected to NGO intervention and demanded that the government pay more attention to the programmes.
2. The government should regulate entry of different NGOs to the village. There has to be a restriction on too many NGOs trying to intervene in similar programmes. Only those NGOs should be encouraged to intervene in bigger programmes, who were familiar with the social mileu (gender and other equity concerns) and had already established their credibility in the area.
3. The policy of financial assistance/compensation should be changed. For example the relocation entitlement norms should be based on the nature of damage and not the economic class of the household. Similarly, compensation packages could be designed according to the economic class of the people, e.g the rich and those who can construct their own houses should be given the least. Higher amounts could be given to widows, destitute women, poor families and the aged who had no kin-support. However, technical assistance could be provided to all irrespective of caste, class and community affiliations. In the relief phase all should be included. Criteria for differential assistance should be strictly followed in a transparent manner.
4. The involvement of the NGOs in the rehabilitation activities viz shelter construction should to be in line with the broad government guidelines and policies which were developed through joint consultations including NGOs. The latter should not have dissimilar shelter packages, which may cause latent tensions and even conflicts among the people in future.

Given the magnitude of the rehabilitation works and limited capacity of the NGOs, the most effective contributions of the NGOs could be:

(a) Facilitating the formation of village rehabilitation committees and their continued operation;
(b) Need assessment and monitoring progress of the rehabilitation works;
(c) Two-way information dissemination regarding rehabilitation i.e. from the villagers to the government and other agencies engaged in rehabilitation and vice versa;
(d) Advocacy work – lobbying and pressurizing the government for appropriate policy formulation and rehabilitation programmes. Towards this the NGOs have to come together and develop their networks like Abhiyan to be effective in their activities. This will facilitate accountability and transparency in relief and rehabilitation works.

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Notes

[1] *Bhoonga* is a round shaped housing structure comprising a single room. They are the traditional housing of the rural population of Kachchh. It was observed that these structures were less damaged during the earthquake. Women particularly preferred the *bhoonga* housing design because of its functional nature.

[2] The speech was taken from the field notes of a Post-graduate student of the Institute of Rural Management who was in a village in Rapar undergoing his training (Jan 2002) for rural orientation as part of requirement for the Masters programme.

[3] The Kachchh Nav Nirman Abhiyan popularly known as the Abhiyan is a network of 29 NGOs that has been working in Kachchh for the past 5 years. It has contributed to a great extent to the rehabilitation policies and programmes in Kachchh. Abhiyan periodically brings out a document called "Coming Together" which was a compilation of all organizations working towards rehabilitation of Kachchh.

REFERENCES

1. Abhiyan/UNDP/GSDMA (2002). Coming Together (January and September editions), Bhuj.
2. Mahadevia, D., (2001). "Privatising Earthquake Rehabilitation", *Economic and Political Weekly*, 36 (39): 2670-2673.
3. Gujarat State Disaster Management Authority (2001). Government Order and Resolutions, Gandhinagar.

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RESEARCH ARTICLE

Molecular Interaction Study Using Ultrasonic Technique of Binary Liquid Solution

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ABSTRACT

The density and viscosity have been measured at different temperatures i.e. at 303 K, 308K, 313 K, 318K and 323K for binary liquid solution of polymer dextran and aqueous 6(M) urea. Ultrasonic speed (U) in the solution have also been measures at four different frequencies i.e. 1MHz, 5MHz, 9MHz, and 12MHz.The acoustic parameters such as adiabatic compressibility , acoustic impedance , relaxation time , intermolecular free length and Gibbs free energy , data have been considered from the measuredvalue. Thermo acoustic data are used to investigate the interaction in the liquids. Depending on these parameters, the interaction present in the solution such as the association of dipole-dipole, hydrogen-bonding, acceptor-donor, and electrostriction is analysed.Above parameters are utilized to get to and clarify the structure and quality of the molecular interaction of dextran with urea.

Keywords: Dextran, Binary liquid solution, Molecular interaction, Dipole-dipole association, Ultrasonic technique.

INTRODUCTION

The adaptable non-destructive technique, Ultrasonic is highly useful for the investigation of various physic-chemical properties such as adiabatic compressibility (β), acoustic impedance (Z), relaxation time (τ), intermolecular free length (L_f) and Gibb's free energy (ΔG). In science the ultrasonic approach is commonly used. In this the sound wave is directly interacting with the particle[1-2]. The molecular interactions and the structural behavior of molecular and their mixtures can be recognized with the help of ultrasonic studies. Using the measured values of ultrasonic velocity jointly with density and viscosityat five various temperatures ranges from 303 K to 323K and at four different

frequencies i.e. 1, 5, 9, 12MHz, the thermodynamic factors such as (β), (Z), (τ), (L_f) and (ΔG)can be determined,for binary solution of dextran (0.5%) and 6(M) urea with distilled water [3].

Dextran is a complex, branched polysaccharide made of numerous glucose atoms made out of chains of fluctuating length from 10 to 150 kilo Daltons. Dextran, a water-soluble polymer, is an α-D-1, 6-glucose connected glucan with side chains l-3 connected to the backbone units of the polymer. Dextran have incredible potential for applications in different nourishment items as conditioners, stabilizers, bodying specialists or related uses. It is used as drugs, especially as blood plasma volume expander [4-6]. Urea is a mineral that is only stable in an arid environment. The structure of urea the carbon is attached to oxygen by a double bond where as it is attached to two NH_2 with single bond each. Urea is utilized in numerous multi-segment strong compost details. Urea is exceptionally dissolvable in water and is in this manner likewise entirely appropriate for use in manure arrangements.

EXPERIMENTAL AND THEORETICAL WORK

Materials

The solution prepared in distilled water as a solvent for preparing the dextran solution at different concentrations. Dextran of MW-70,000 Da utilized as a solute, Solvent 6(M) urea used in this state throughout the experiments.

Measurements

(a) Velocity Measurement:-

The interferometer produces precise and reliable data, from which one can determine the velocity of ultrasonic sound in a liquid medium. Operational frequencies ranging from 1 to 12 MHz has been utilized to calculate the ultrasonic velocity. The ultrasonic measuring cell has a double walled brass cell with chromium plated surfaces which consist of thecapacity of 10 ml. An electronically worked advanced steady temperature shower provided by M/s Mittal Enterprises, New Delhi, (Model SSI-03spl) working in the temperature range -10 ^{0}C to 85 ^{0}C with an precision of ± 0.1K has been utilized to circulate water through the external jacket of the two-fold walled estimating cell containing the test fluid.

(b) Density (ϱ) Measurement:-

The ϱ of the solution were estimated using a 10ml Pycnometer bottle. The Pycnometer with the investigational solution was submerged in a temperature-regulated water shower.

(c) Viscosity (η) measurement:-

The η of the solution were estimated using Ostwalds viscometer standardized with distilled water. The Ostwald's viscometer with the investigational solution was submerged in a temperature-regulated water shower. The time of flow was measured using an advanced stopwatch with a precision of 0.01 s

Theory

a)Velocity(U):-

The expression used to determine the ultrasonic velocity is

$$U = 2d/T \text{ (m/s)}$$

$$\text{Or.} \quad U = 2d \times v$$

$$\text{Or,} \quad U = \lambda \times v$$

(Here-2d=λ)

Where, v is the frequency of the generator which is used to excite the crystal; (In the present investigation, different frequency frequencies (1MHz, 5MHz, 9MHz and 12MHz interferometer was employed) d- Separation between the reflector and crystal; T. Travel time of the ultrasonic wave.

b) Density (ρ):-

The density was estimated using the equation

$$\rho_{2=} (w_1/w_2)\rho_1$$

Where, w_1 = weight of distilled water, w_2 = Weight of solution, ρ_1 = Density of water, ρ_2 = Density of solution.

c) Viscosity (η):-

The viscosity was calculated using the equation,

$$\eta_2 = \eta_1 (t_2/t_1)(\rho_2/\rho_1)$$

Where, η_1 = Viscosity of distilled water, η_2 = Viscosity of solution, ρ_1 = Density of distilled water, ρ_2= Density of solution. t_1 = Time of flow of water, t_2 = Time of flow of solution.

The following thermo acoustic parameters were calculated

a)Acoustic Impedance (Z):

$$Z=\rho.u$$

b) Adiabatic compressibility (β):

$$\beta = 1/\rho u^2$$

c) Intermolecular free length (L_f):

$$L_f=(K_T/\rho\, u^{1/2})$$

d) Relaxation Time (τ):

$$\tau = (4/3)\ (\eta\ .\beta)$$

e) Gibb's free energy (ΔG):

$$\Delta G = k_B T \ln (KT\tau/h)$$

Where K_T = (93.875+0.375T) x$10^{-8}$is a temperature dependent constant *T*is the absolute temperature, *k* is the Boltzmann's constant and *h* is the Planks constant.

RESULTS AND DISCUSSION

The ρ and η of dextran with sodium hydroxideat temperature 303K, 308K, 313K, 318K and 323Kare represented in Table-1 The Ultrasonic speed increases with rise in temperature at a particular frequency (fig.1), which suggests that disruption of water structure is enhanced with the addition of solvent (urea) and the solutes (dextran). The association is due to dipole are induced due permanent dipoles are present in the water molecules suggest that reduction in intermolecular forces due to rise inthermal energy of the system.Ultrasonic velocity decreases with increase in frequency for a given temperature[7-8]. The decrease in speed is an indication of existence of weak molecular association between the solute and solvent due to increase in agitation between molecules give rise to decrease in speed at higher frequency (12MHz) the trend is reverse (fig.2). The β falls with rise in temperature at a given frequency and β rises with rise in frequency at a given temperature. This type of behaviour may be due to breaking up of associated clusters of urea and dextran releasing several dipoles, which in turn induces dipole moment in urea resulting dipole- induced dipole interaction between them. The decrease in Z is an indication of existence of weak molecular association between the solute and solvent in both temperature and frequency rises, leads to increase agitation between molecules give rise to decrease in Z at higher frequency (12MHz) the trend is reverse (fig.2). This supports the possibility of weak interaction between unlike molecules at a given temperature and frequency[9]. The fig.7 indicates the τ drops with rising temperature. This is due to the increase in temperature causesnumber of collision and hence decreasing the collision time leading to less τ. The variation of τ with frequency is almost parallel to frequency axis (fig.8) indicating very small change in τ with increase in frequency [10]. Intermolecular attractions between the components is in binary mixture is measured by Lf. Weakling and strengthen of intermolecular attraction is indicated by the increase or decrease in free length. As theultrasonic velocity increase due to the increases in temperature, the Lfhas to decrease. The variation of Lf with frequency is almost parallel to frequency axis (fig.10) indicating very small change in Lfwith increase in frequency[11] The ΔG reveals closer packing of the molecules due to the H-bonding of unlike molecules in the solutions. The ΔG decreases with temperature rise suggesting that less time is required for the cooperative process or the rearrangement of molecules

in the solution decreases the energy leading to dissociation. The variation of ΔG with frequency is almost parallel to frequency axis (fig.12) indicating very small change in ΔGwith increase in frequency [12].

CONCLUSION

The structural properties of solutions were determined. Temperature change provided molecular interactions such as solvent-solvent and dipole-dipole interactions.

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REFERENCES

1. Bhandakkar V.D., Chimankar O.P., Pawar N.R. (Ultrasonic study of molecular interactions in some bio liquids) J. Chem. Pharm. Res., 2010; 2(4): 873-877.
2. Mahapatra A.P., Samal R.K., Samal R.N. and Roy G.S., Evaluation of thermo-viscosity parameters of dextran in polar and nonpolar solvent, *J. Appl. Poly. Sci.*, 81(2001) 440-452.
3. Panda Subhraraj, Evaluation of ultrasonic parameters in binary solution of dextran and urea at various concentration and temperatures.Indian Journal of Natural Sciences.2020,10(59), 18552-18557
4. Chen Hong, Konofagou Elisa E. (The size of blood– brain barrier opening induced by focused ultrasound is dictated by the acoustic pressure.) Journal of Cerebral Blood Flow & Metabolism, 2014; 34 (7): 1197.
5. Jeanes A., Haynes W.C., C. Wilham A., Rankin J.C., Melvin E.H., Austin M. J., Cluskey J. E., Fisher B.E., Tsuchiya H.M. and RistC.E.,Characterization and classification of dextrans from ninety-six strains of bacteria, *J. Am. Chem. Soci.*, 76 (1954) 5041-5052.
6. Armstrong J.K.,Wenby R.B., Meiselman H.J. and Fisher T.C., The hydrodynamic radii of macromolecules and their effect on red blood cell aggregation, *Biophysical J.*, 87 (2004) 4259-4270.
7. Panda Subhraraj and Mahapatra Achyuta Prasad,Molecular interaction of dextran with urea through Ultrasonic technique,Clay Research,2019, 38(1) 35-42
8. Panda Subhraraj and Mahapatra Achyuta Prasad, Intermolecular interaction of dextran with urea, International Journal of Innovative Technology and Exploring Engineering 2019, 8(11), 742-748.
9. Pawar N. R., Chimankar O. P. Bhandakkar V. D. and Padole N. N., Study of binary mixtures of acrylonitrile with methanol at different frequencies, *J. Pure Appl. Ultrason.*, (2012), 49.11-13.
10. Panda Subhraraj., Ultrasonic study on dextran in aqueous media at 313 K at different frequencies, Adalya Journal,2020,9(3), 456-462
11. Panda Subhraraj and Pradhan Shibashis, Molecular Interaction of Dextran with (1N) NaOH through Ultrasonic Technique, Indian Journal of Natural Sciences2020, 10(59), 18340-18345
12. Praharaj MK, Satapathy A, Mishra P and Mishra S. Ultrasonic studies of ternary liquid mixtures of N-Ndimethylformamide, nitrobenzene, and cyclohexane at different frequencies at 318 K Journal of Theoretical andApplied Physics 2013; 7:23-6

Table: 1-The values of density (ρ) and viscosity (η) at 303K, 308K, 313K and 318K ofsolution.

T in kelvin	(ρ) $Kg.m^{-3}$	(η) 10^{-3} $N.s.m^{-2}$
303	1078.75	1.086
308	1076.75	1.036
313	1075.40	0.963
318	1072.57	0.900
323	1069.00	0.834

Table: 2- values of U and β at different temperature and frequencies

T in kelvin	Velocity (U) m.s^{-1}				Adiabatic Compressibility β (10^{10} m^2 N^{-1})			
	1MHz	5MHz	9MHz	12 MHz	1MHz	5MHz	9MHz	12 MHz
303	1624	1619	1616	1617	3.5149	3.5388	3.5497	3.5454
308	1626	1621	1618	1619	3.5127	3.5344	3.5475	3.5432
313	1627	1623	1620	1621	3.5128	3.5323	3.5432	3.5389
318	1629	1625	1622	1624	3.5135	3.5308	3.5438	3.5351
323	1632	1628	1625	1626	3.5122	3.5295	3.5428	3.5382

Table: 3- values of *Z* and τ at different temperature and frequencies

T in kelvin	Acoustic impedance (Z) (×10^4)kg·m^2·s^{-1})				Relaxation time (τ)(x 10^{10})s			
	1MHz	5MHz	9MHz	12 MHz	1MHz	5MHz	9MHz	12 MHz
303	1.752	1.746	1.743	1.744	5.091	5.126	5.142	5.135
308	1.751	1.745	1.742	1.743	4.853	4.883	4.901	4.895
313	1.750	1.745	1.742	1.743	4.508	4.533	4.547	4.542
318	1.747	1.743	1.740	1.742	4.216	4.237	4.253	4.242
323	1.745	1.740	1.737	1.738	3.903	3.922	3.937	3.932

Table: 4- values of L$_f$ and ΔG at different temperature and frequencies

T in kelvin	Intermolecular free length (L$_f$)(10^{-10} m)				Gibb's free energy (ΔG)(10^{-20} K.J.mol^{-1})			
	1MHz	5MHz	9MHz	12 MHz	1MHz	5MHz	9MHz	12 MHz
303	3.720	3.732	3.738	3.736	212.13	213.36	213.92	213.70
308	3.751	3.763	3.770	3.767	209.82	210.96	211.64	211.41
313	3.783	3.794	3.800	3.797	202.41	203.45	204.03	203.80
318	3.816	3.825	3.833	3.828	195.89	196.83	197.53	197.06
323	3.848	3.857	3.864	3.862	187.06	188.01	188.74	188.49

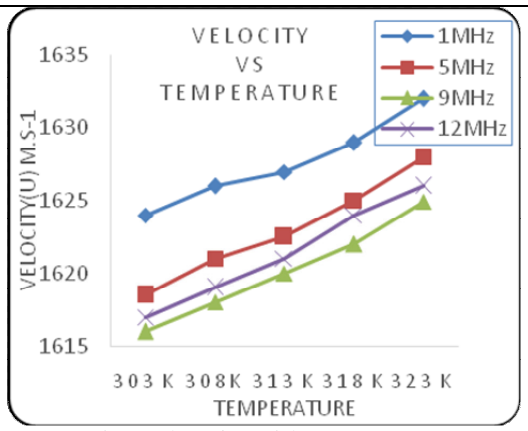

Fig.-1 Plot of U with temperature

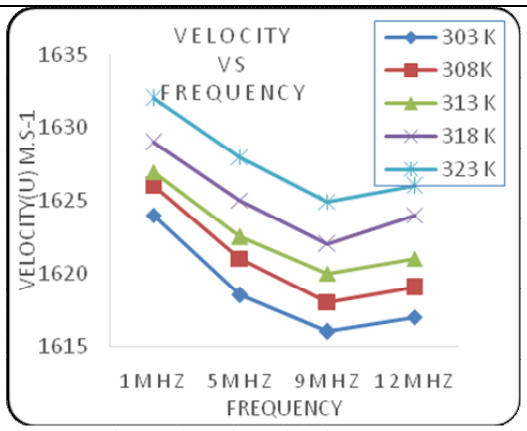

Fig.-2 Plot of U with frequency

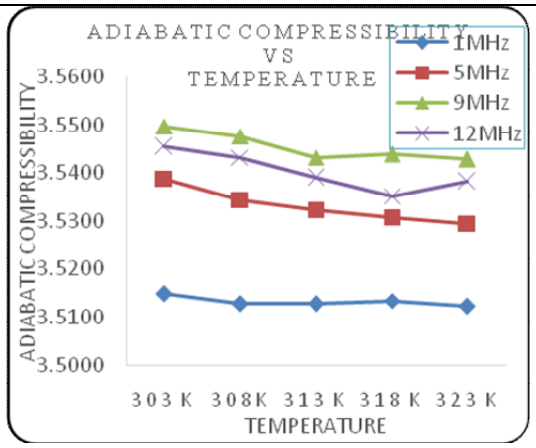

Fig.-3 Plot of β with temperature

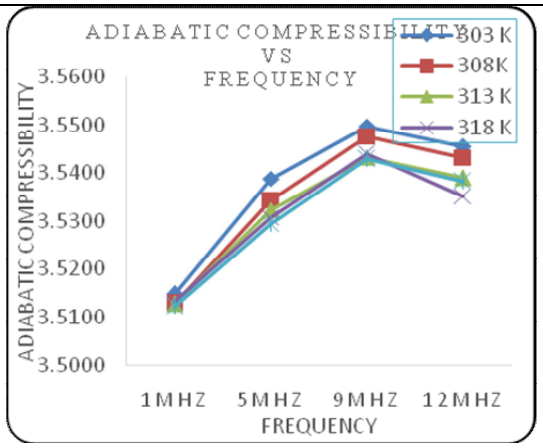

Fig.-4 Plot of β with frequency

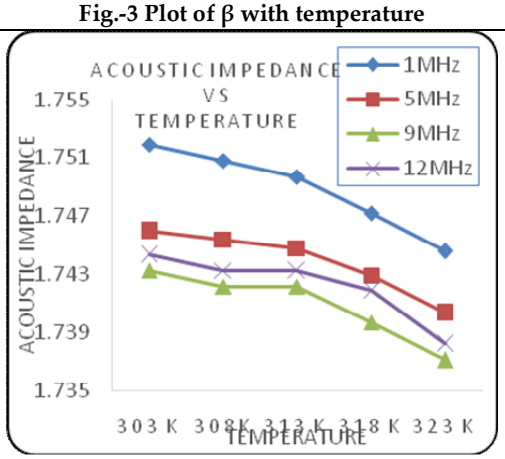

Fig.-5Plot of Z with temperature

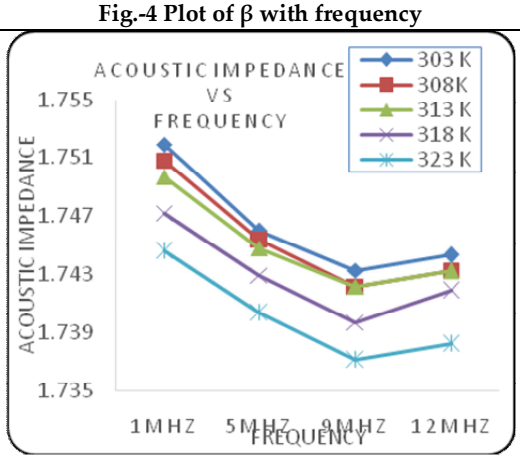

Fig.-6Plotof Z with frequency.

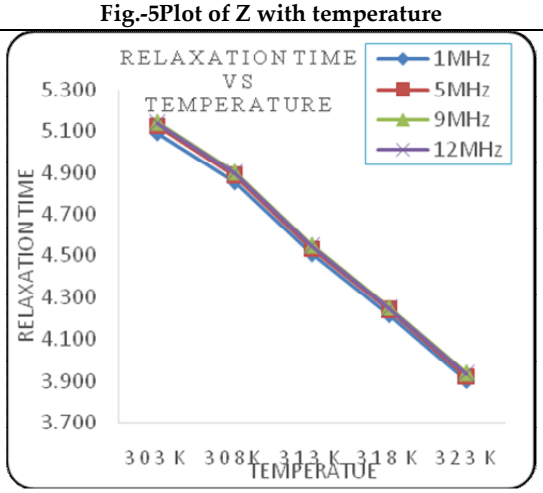

Fig.-7 Variation of τ with temperature

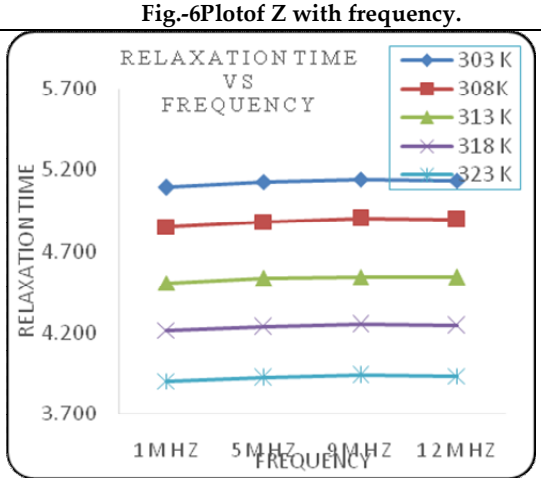

Fig.-8 Variation of τ with frequency

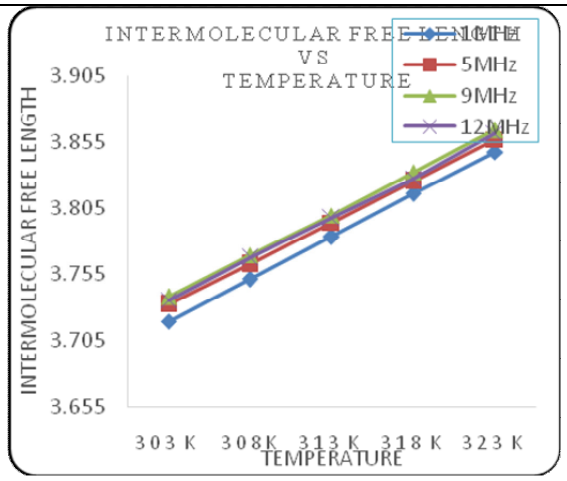

Fig.-9Plot of *Lf*with temperature

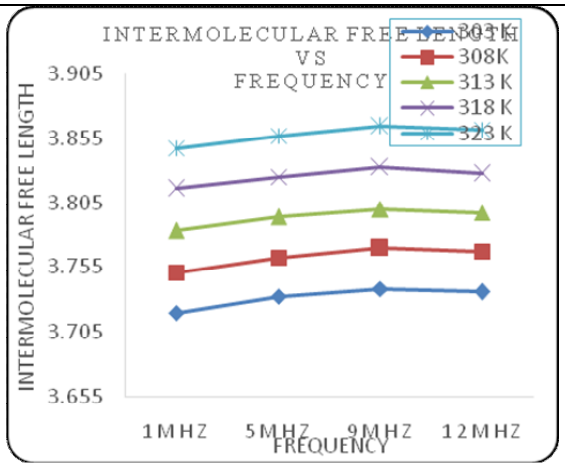

Fig.-10Plot of *Lf*with frequency

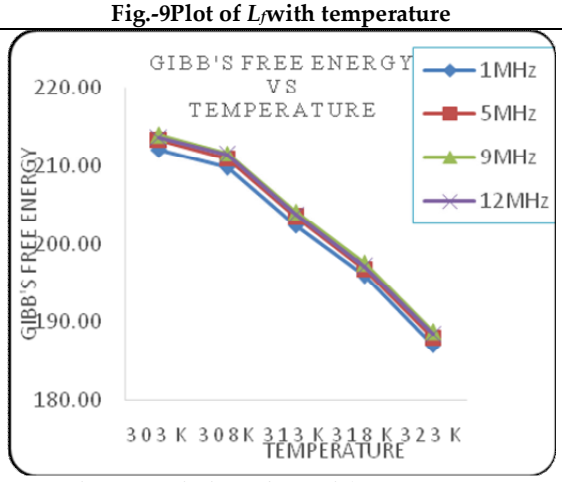

Fig.-11 Variation of ΔGwith temperature

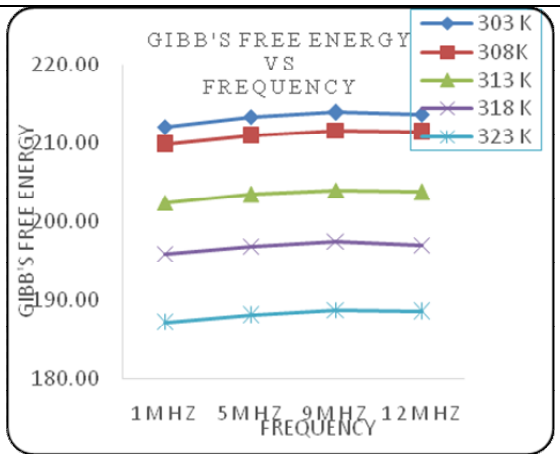

Fig.-12 Variation of ΔG with frequency

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RESEARCH ARTICLE

Determination of Thermo Acoustical Parameters of Dextran with Glycine at 303 K and at Frequency 9MHz

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ABSTRACT

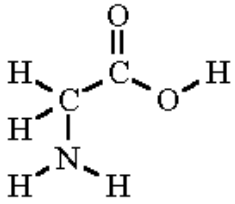
The ultrasonic speed (u), density (ϱ) and viscosity (η) at 303 K have been measured in the liquid solution of dextran over range of concentrations (0.1%, 0.25%, 0.50%, 0.75%, and 1%) and glycine. The variousacoustical parameters such as ,acoustic impedance (Z), adiabatic compressibility (β), intermolecular free length (L_f), relaxation time (τ) , Gibb's free energy(ΔG) have been computed from three basic parameters ultrasonic speed (u), density (ϱ) and viscosity (η). The results have been presented in the light of the molecular interaction among solute and solvents molecules. The molecular interactions like electrostriction, acceptor-donor association, dipole-dipole association and hydrogen bonding have been analyzed based on these parameters. The properties of solution can be altered within a reasonable range by varying the concentration till an optimum value of some desired parameter is attained.

Keywords: ultrasonic speed, density,viscosity and dipole-dipole association.

INTRODUCTION

The study of molecular interaction in liquid solutions plays an important role in the development of molecular sciences[1-2]. The ultrasonic technique, is being mostly used in the study of molecular interaction in liquid state due to their simplicity and accuracy. As these techniques are nondestructive, it plays an important tool for basic research in Physics, Chemistry, Material Science, Biology, medical science and forensic science. The present investigation is related on thermo acoustical properties of polymer dextran with glycine. The thermo-acoustical parameters such as acoustic impedance (Z), adiabatic compressibility (β), intermolecular free length (L_f), relaxation time (τ) , Gibb's free energy(ΔG) of polymer dextran 70,000 Da at various concentration i.e. 0.1, 0.25, 0.50, 0.75 and 1% in solvent glycine at constant temperature and frequency at 303K and 9MHzrespectively have been calculated.Dextran, a water soluble

polymer, has occupied a separate area of investigations by researchers[3-6]. It is used widely in the manufacture of blood plasma expanders [7-8]. Glycine is an organic compound with the formula $HO_2CCH_2NH_2$. It is an amino acid and is found often in small quantities in proteins. Glycine can be found in myoglobin and hemoglobin



Structure of Glycine

The body uses glycine to make proteins, and widely used in the biological activity of our body.In view of the importance of dextran and glycine, a systematic study of it with glycine has been undertaken in the present study.

EXPERIMENTAL SETUP

Materials

The aqueous solution 2(M) glycine with dextran of 70,000 Da is prepared for preparing dextran solution. Dextran of 70,000 Da used as solute at different concentration (0.1, 0.25, 0.50, 0.75 and 1%) [9-10]

Measurements

The Methods adopted for measurement of velocity, density and viscosityare same as mypreviousarticle [11].

Theoretical Aspect

The ϱ, η and U, have been measured and using these measuredvaluethe parameters β, Z, τ, L_f and ΔG, were evaluated using standard formula [9].

RESULTS AND DISCUSSION

It is observed that, ultrasonic velocity rises with increase in concentration at 303K as shown in figure-1. Variation in the velocity is due to self-association of the glycine and water atoms and dipole-induced dipole interaction among the component systems, which is concentration dependent. With increase in dextran concentration, dipole-induced dipole interaction increases making the system less compressible resulting increase in velocity. It is observedfromfigure-2 that values of acoustic impedance increase with increase in concentration of dextran as in velocity which is in agreement with the theoretical requirement. Increase in impedance with solute concentration can be attributed to the effective solute solvent interactions [8].As expected β drops with rise in concentration of dextran which shows a reverse trend to velocity graph in figure-3 This behavior may be due to breaking up of associated clusters of dextran releasing several dipoles, which in turn induces dipole moment in glycine resulting dipole-induced dipole interaction [10].From figure-4 it is observed that the value of intermolecular free length decreases steadily with increase of concentration of dextran. This indicates the significant dipole–induced dipole interaction between solute and solvent due to which structural arrangement is affected. Dextranhave higher molar volume, therefore, molar volume of dextran part rises with increase inconcentration of dextran and occupies larger spatialarrangement in the molecular core of the solution[11-12] whichleaves less intermolecular space in between the associatedstructure present in the system. Figure-5τ increase with rise in concentration of dextran. Such situation suggests that, the molecules getrearranged due to co-operation process [13-14]. The Gibbs free energy (ΔG) rises with the rise in concentration of dextranas shown in figure-6. An increasing value of ΔG recommends that the

nearerattitude of unlike particles is due to hydrogen bonding. The rise in ΔG leads tosmaller time for the rearrangement of molecules in the mixture.

CONCLUSION

The evaluated values of ultrasonic speed and other derived parameters indicate the presence of molecular interaction between component molecules at constant temperature and for frequency 9 MHz.. Summarizing the trends and variation of thermodynamic parameters with concentration of the ultrasonic wave has been studied in detail which will give us an idea about the nature of molecular interactions between the solute (dextran) and solvent (glycine).

ACKNOWLEDGEMENTS

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REFERENCES

1. François P.,André M.,Pierre M.,(1986) Microbial polysaccharides with actual potential industrial applications,Biotechnology Advances ,4, 2, 245-259.
2. Jeanes, A.; Haynes, W.C.; C. Wilham, A.; Rankin, J.C; Melvin, E.H.; Austin, M. J.; Cluskey, J. E.; Fisher, B.E.; Tsuchiya, H.M.; Rist, C.E. (1954),Characterization and Classification of Dextrans from Ninety-six Strains of Bacteria. Journal of American Chemical Society, 76 (20),5041-5052.
3. Arond L.H.; Fran, H.P.Molecular weight, molecular weight distribution and molecular size of a native dextran. Journal of Physical Chemistry, 58(11), (1954), 953-957.
4. Armstrong, J. K.; Wenby, R. B.; Meiselman, H. J.; Fisher, T. C..(2004), The Hydrodynamic Radii of Macromolecules and Their Effect on Red Blood Cell Aggregation. Biophysical Journal, 87, 4259-4270.
5. Pribush, A.; Zilberman-Kravits, D.; Meyerstein, N..(2007), The mechanism of the dextran-induced red blood cell Aggregation. European Biophysical Journal, 36,85-94.
6. Barshtein, G.; Tamir, I.; Yedgar, S.,(1998), Red blood cell rouleaux formation in dextran solution: dependence on polymer conformation. European. Biophysical Journal, 27, 177-181.
7. Castellanos Gil, E. E.; IraizozColarte, A.; El Ghzaoui, A.; Durand, D.; Delarbre, J.L.; Bataille, B. (2008), A sugar cane native dextran as an innovative functional excipient for thedevelopment of pharmaceutical tablets. European Journal of Pharmaceutics and Biopharmaceutics, 68,319-329.
8. Mahapatra,A.P.,Samal,R.K.,Samal,R.N.,&Roy,G.S.,(2001),Evaluation of Viscosity-Molecular Weight Constant (K), Short Range Parameter (A) and Long Range Parameter (B) of Dextran in Polar Solvents. Physics chemistry of liquids, 39(3) 343-356.
9. Panda,S., Mahapatra, A,P International Journal of Pure and Applied Physics. ISSN 0973-1776 Volume 12, Number 1 (2016), pp. 71-79
10. Panda,S.,Mahapatra, A,P.,(2019),Intermolecular Interaction of Aqueous Dextran with Urea,International Journal of Innovative Technology and Exploring Engineering,8(11),742-748
11. Panda,S.,Mahapatra, A,P.,(2015),Molecular interaction studies of aqueous Dextran solution through ultrasonicmeasurement at 313K with different concentration and frequencyScholars Research Library,Archives of Physics Research, 6 (2),6-12
12. Panda,S.,Mahapatra,A.P.,(2014) ,Variation of thermo-acoustic parameters of dextran with concentration and temperatureJournal of Chemical and Pharmaceutical Research,6(10), 818-825.

13. Mahapatra, A.P., Samal, R.K., Samal, R.N.,& Roy, G.S.,(2001),Evaluation of thermo-viscosity parameters of dextran in polar and nonpolar solvent. Journal applied polymer science. ,81(2), 440-452 .
14. Panda, S.,Mahapatra,A.P.,(2015),Study of Acoustic and Thermodynamic Propertiesof Aqueous Solution of Dextran at DifferentConcentration and Temperature through UltrasonicTechniqueInternational Journal of Science and Research (IJSR), International Symposium on Ultrasonics,503-508.

Table 1 Values of ϱ and ηof solution.

T (kelvin)	Concentration									
	0.10%		0.25%		0.50%		0.75%		1%	
	ρ $Kg.m^{-3}$	η 10^{-3} $N.s.m^{-2}$	ρ $Kg.m^{-3}$	η 10^{-3} $N.s.m^{-2}$	ρ $Kg.m^{-3}$	η 10^{-3} $N.s.m^{-2}$	ρ $Kg.m^{-3}$	η 10^{-3} $N.s.m^{-2}$	ρ $Kg.m^{-3}$	η 10^{-3} $N.s.m^{-2}$
303	1053.50	1.079	1054.69	1.093	1055.48	1.129	1056.27	1.233	1057.86	1.251

Table 2 Values of U and Zof solution at 303K temperature.

Conc.	**(U) m/s**	**(Z) 10^6 kg·m²·s⁻¹)**
0.10%	1600	1.686
0.25%	1601	1.689
0.50%	1602.45	1.691
0.75%	1605	1.695
1%	1606	1.699

Table 3 Values of β and $L_f$of solution.at 303Ktemperature

Conc.	β ($10^{-10}N^{-1}.m^2$)	L_f(10^{-10} m)
0.10%	3.708	3.821
0.25%	3.699	3.816
0.50%	3.690	3.811
0.75%	3.675	3.804
1%	3.665	3.798

Table 4 Values of τ and ΔGof solution at 303 K temperature

Conc.	(τ)(10^{-13} s)	(ΔG)10^{-20}kJ·mol⁻¹
0.10%	5.334	220.607
0.25%	5.389	222.451
0.50%	5.553	227.913
0.75%	6.043	243.286
1%	6.114	245.394

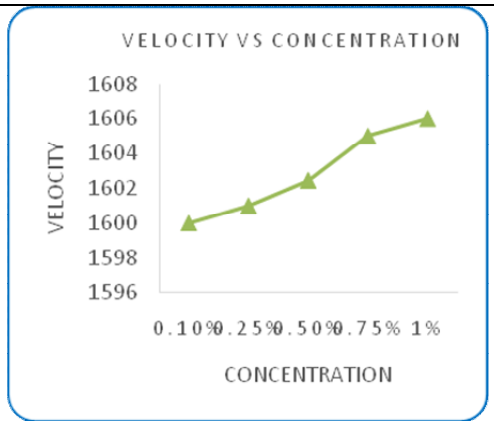

Fig.1 Variation of U with concentration

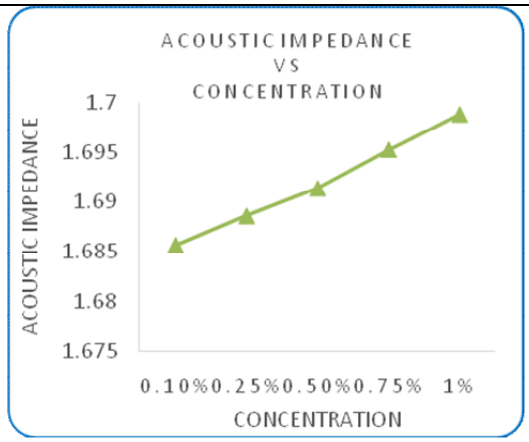

Fig.2 Variation of Z with concentration

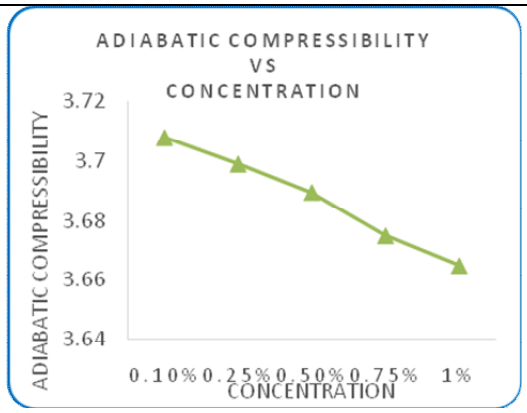

Fig.3Variation of β with concentration

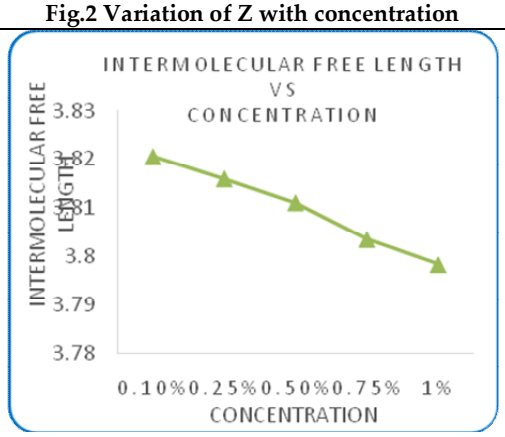

Fig.4Variation of L*f*with concentration

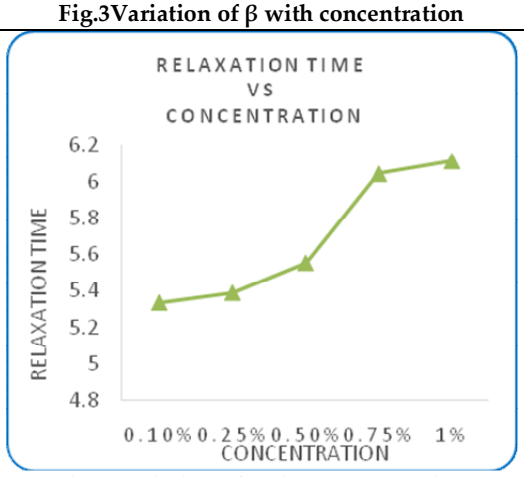

Fig.5 Variation of τwith concentration

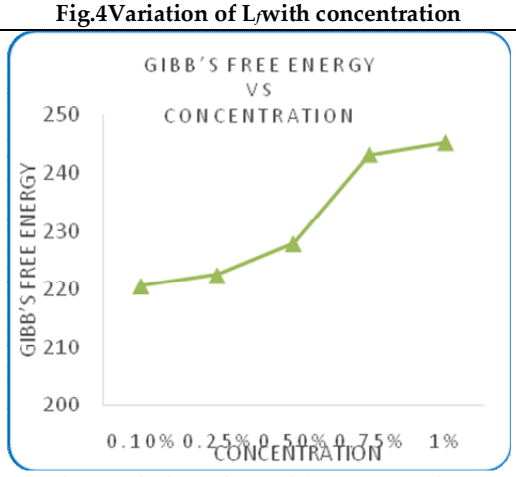

Fig.6Variation of ΔGwith concentration

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RESEARCH ARTICLE

Physico-Chemical Properties of Edible Oils through Ultrasonic Investigation

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ABSTRACT

This work presents an ultrasonic method to measure the physico-chemical properties of edible oils. Over last decade less work has been done in evaluation of physico-chemical for a wide variety of edible oils using ultrasonic technique. It is important because of their extensive use in bio-engineering, food engineering, pharmaceutical industries, process industry, textile industries and nuclear energy industries. Ultrasound can be used to determine the dynamic rheology and composition of oils, the oil contents. Ultrasonic velocity and acoustical parameters have useful in investigation of structure of oils and interaction between the molecules. The ultrasonic velocity, density viscosity,adiabatic compressibility and intermolecular free length have been measured at fixed frequency 4MHz.at temperature 30 ^{0}C, 35^{0}C, 40^{0}C and 45 ^{0}C. The influences of temperature on physic-chemical properties are analyzed. The present study throws light in understanding these oils with regard to their purity and data presented will be highly useful to identify the adulteration in oils. The influences of temperature on physic-chemical properties are analyzed.From the experimental data acoustic and thermo dynamical parameters have been calculated. In this present work the parameter adiabatic compressibility (β), and intermolecular free length (L_f) have been computed using the standard relations.

Keywords: ultrasonic method, physico-chemical, edible oils

INTRODUCTION

The structure of associated liquids has been subject of continuous study. Since the recognition of H bonding, though a number of methods are available, the ultrasonic method is used by many as it is relatively easy, involving less number of measurement parameters as well as few assumptions. Further ultrasonic methods find wide application in fundamental research, in Pharmaceutical industry and Defense. It is also a universally accepted technique to study the physical-chemical properties at the macro level of the liquids, liquid mixtures, electrolytic solutions and

polymeric solutions. Measurement of ultrasonic velocity has been adequately employed in understanding the molecular interactions in pure, binary, and higher order multicomponent liquid mixtures. The propagation of ultrasonic velocity in a medium is a thermodynamic property and has come to be recognized as a very specific and unique tool for predicting and estimating various physico-chemical properties of the systems under consideration [1]. The propagation of ultrasonic waves in oils depends on its visco-elastic behavior and density which significantly affected with change in temperature and frequency [2-3] .Therefore the application of low intensity ultrasound acting as a high frequency dynamic mechanical deformation applied to oils, can monitor the changes in acoustic and thermodynamic properties associated with it. In this thesis the bulk properties like density, viscosity and ultrasonic velocity are measured at four different temperatures like 303 K, 308 K, 313 K, and 318 K at frequency 4MHz.These experimental data has been used to calculate the acoustic and thermo dynamical parameter such as adiabatic compressibility (β), and intermolecular free length (L_f).The densities (ϱ) of the oils, using specific gravity bottle, ultrasonic speed (U) by using a single-crystal variable-path multi-frequency ultrasonic interferometer and viscosity (η) by using, Ostwald viscometer are used[4-5] .From the experimental data acoustic and thermo dynamical parameters have been calculated. In this present work the parameter adiabatic compressibility (β), and intermolecular free length (L_f) have been computed using the standard relations. The variation of ultrasonic velocity and acoustical and thermo dynamical parameter with different temperature leads to the analysis of intermolecular interaction among the oil samples [6-7].

MATERIALS

Different standard edible oil like mustard, groundnut, palmolein & sunflower were collected from business units as samples to compare & investigate different characteristics & dynamic properties.

Experimental Details

Speed

The speed of the ultrasonic wave in the solution has been measured utilizing an ultrasonic interferometer, working at 11 various frequency supplied by M/s Mittal Enterprises, New Delhi (Model M-84). The measuring cell of the interferometer is a specially structured twofold walled vessel with an arrangement for temperature constancy. . An electronically worked advanced steady temperature shower provided by M/s Mittal Enterprises, New Delhi, (Model SSI-03spl) working in the temperature range -10 ^{0}C to 85 ^{0}C with an precision of ± 0.1K has been utilized to circulate water through the external jacket of the twofold walled estimating cell containing the test fluid.

The expression used to determine the ultrasonic velocity is

$$U = 2d/T \text{ (m/s)}$$

Or. $U = 2d \times v$

Or, $U = \lambda \times v$

(Here-$2d=\lambda$)

Where, v is the frequency of the generator which is used to excite the crystal; (In the present investigation, the frequency 4MHz interferometer was taken) d- Separation between the reflector and crystal; T. Travel time of the ultrasonic wave.

Density (ρ)

The ϱ of the solution were estimated using a 10 ml Pycnometer bottle. The Pycnometer bottle with the transformer oil was submerged in a temperature-controlled water shower at 30 °C.35°C, 40 °C and 45°C.The ϱ was estimated using the equation

$$\rho_1 = (w_2/w_1)\,\rho_2$$

Where, w_1 = weight of distilled water, w_2 = Weight of investigational solution, ϱ_1 = Density of water, ϱ_2 = Density of oil samples.

Viscosity (η)

The viscosities of the solution were estimated using Ostwald's viscometer standardized with distilled water. The Ostwald's viscometer with the transformer oil was submerged in a temperature-controlled water showerat 30 °C.35°C, 40 °C and 45°C.The time of flow was measured using an advanced stopwatch with a precision of 0.01 s. The η was calculated using the equation,

$$\eta_2=\eta_1 (t_2/t_1)(\rho_2/\rho_1)$$

Where, η_1 = Viscosity of distilled water, η_2 = Viscosity of solution, ρ_1 = Density of distilled water, ρ_2 = Density of oil samples. t_1 = Time of flow of water, t_2 = Time of flow of oil samples

Theoretical Aspect

The information of ultrasonic speed, ρ, and η lead to the determination of different thermo-acoustical parameters, using standard equation.

Adiabatic compressibility $\beta = 1/\rho u^2$

Intermolecular free length $L_f= (K_T/\rho\, u^{1/2})$

RESULTS AND DISCUSSIONS

The density of oil samples is given in Table 1.The viscosity of the oil samples is listed in table 2.The velocity of oil samples is listed in the table 3.The adiabatic compressibility of oil samples is given in table 4 and variation between adiabatic compressibility and temperature is shown in fig.4.The inter molecular free length of oil samples is given in table 5 and variation between inter molecular free length and temperature is shown in fig.6. According to the molecular theory, when a liquid is heated the molecules move apart i.e. it expands, the number of molecules or mass remains the same but the volume increases and as a result the density and viscosity decrease in all the oils. Density and viscosity decrease with increase in temperature indicates decrease in inter molecular forces due to increase in thermal energy of the system. This causes an increase in volume and hence decreases in density and viscosity (fig.1 and fig.2). It is observed that, ultrasonic velocity decreases with increase in temperature (fig.3). This is due to the structural changes occurring in the oils resulting in increase of intermolecular forces. Which is an indication of existence of strong molecular dissociation between the components molecules [8]. The variation of adiabatic compressibility (β) is increases with increase in temperature of different oils (fig.4).Adiabatic compressibility (β) is a measure of intermolecular association or dissociation or repulsion. It also determines the orientation of the component molecules. The structural arrangement of the molecule affects the adiabatic compressibility The decrease in adiabatic compressibility indicates enhancement of degree of association among the oil molecules,Indicates the more fat contains The decrease in adiabatic compressibility brings the molecules to a closer packing resulting into a decrease of intermolecular free length. The decrease in the values of adiabatic compressibility strengthens the strong molecular association between the unlike molecules through dipole-dipole interaction [9]. Inter molecular free length increases with increase in temperature (fig.5). As the temperature increases it leads to the less ordered structure and more spacing between the molecules due to increase in thermal energy of the system which increases in volume expansion and hence increase in inter molecular free length[10].

CONCLUSION

From the above studies, the nature of forces between molecules such as hydrogen bonds, charge transfer complexes, breaking of hydrogen bonds and complexes had been interpreted. Intermolecular forces are weak. Structural characteristics of the components arising from geometrical fitting of one molecules in to another due to the difference in shape and size of the molecules and free volume.

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REFERENCES

1. S.Panda, and A.P.Mahapatra. Acoustic and ultrasonic studies of dextran in 2(M) glycine-variation with frequencies and concentrations.International Journal of Pure and Applied Physics 12(1), 71-79,2016.
2. K Rajagopal, and S Chenthilnath,Molecular interaction studies and theoretical estimation ofultrasonic speeds using scaled particle theory in binary mixtures of toluene withhomologous nitriles at different temperatures, *Thermochimica Acta*, 498(1-2),45-53,2010.
3. S.Panda, and A.P.Mahapatra.Ultrasonic Study of Acoustical Parameters of Dextran Solution with 1(N) NaOH at Different Temperatures and Concentrations.Journal of pure and applied Ultrasonics. 40, 100-105,2018.
4. A P Mahapatra,R K Samal,R N Samal andG SRoy, Evaluation of thermo-viscosity parameters of dextran in polar and nonpolar solvent, *J. Appl. Poly. Sci.*, 8 , 440-452,2001
5. S. Deosarkar, M. Narwade, H. Jahagirdar, K.Khedkar, The measurement of molar refraction and polarizability constants of some substituted sulphonic acids at 303K, *Oriental Journal of Chemistry*; Vol.24 (3), 1135-1137, 2008**.**
6. S Panda and S Mishra ,Analysis of Acoustic Wave Propagation in a Power Transformer oil. gedrag & organisatie review , 33(2),929-934,2020.
7. M. V. Rathnam, Kavita R. Bhanushali, Reema T. Sayed, and M. S. S. Kumar., "Acoustic, thermodynamics and transport properties of binary liquid mixtures of Isopentyl acetate with aryl halides at 303.15 K and 313.15 K," Journal of Molecular Liquids, 173, 35-41,2012.
8. S.Panda, and A.P.Mahapatra ,molecular interaction study using ultrasonic technique of binary liquid solution, journal of xidian university.14(5),485-49,2020.
9. V. DBhandakkar , Shweta Rode,Acoustical studies on molecular interactions in binary
10. liquid Mixtures at 303K, Advs in Appli Sci Res Jour, Pelagia Research Library, 3(5): 3223-3229,2012.
11. G.R.Bedare,V.D Bhandakkar,B.M Suryavanshi,. Studies of Acoustic andThermodynamic Properties of Binary Liquid Mixtures At 308K J. of Chem. & Pharm.Res., 4(2): 1028-1032, 2012.
12.

Table-1 Values of density (ϱ) at different temperatures of different oils

kelvin(T)	Density(ϱ) kg.m^{-3}			
	Palm oil	Groundnut oil	Mustard oil	Sunflower oil
303 K	901.429	908.246	901.913	913.862
308 K	898.423	904.723	899.447	911.037
313 K	894.720	902.501	896.714	908.759
318 K	890.644	898.962	893.354	904.723

Table-2 Values viscosity (η) at different temperatures of different Oils

kelvien (T)	Viscosity(□)10^{-3} N.s.m^{-2}			
	Palmolein oil	Groundnut oil	Mustard oil	Sunflower oil
303 K	66.875	51.291	85.134	47.578
308 K	59.298	45.260	78.018	44.049
313 K	51.562	39.194	52.527	35.378
318 K	42.780	32.500	47.186	30.571

Table-3Ultrasonic velocity (U) at different temperatures of different oils for 4MHz frequency

kelvin(T)	Velocity(*U*) m s^{-1}			
	Palmolein oil	Groundnut oil	Mustard oil	Sunflower oil
303 K	1413.200	1434.000	1438.600	1436.400
308 K	1408.600	1423.000	1430.000	1412.600
313 K	1394.200	1399.800	1408.400	1399.200
318 K	1382.800	1387.800	1395.200	1391.200

Table-4 Adiabatic compressibility (β) of different temperatures of oils for frequency 4MHz

T (kelvien)	Adiabatic Compressibility (β)(10^{-10}N^{-1}.m^2)			
	Palmolein oil	Groundnut oil	Mustard oil	Sunflower oil
303 K	5.555	5.354	5.304	5.357
308K	5.610	5.459	5.501	5.437
313 K	5.750	5.655	5.621	5.622
318 K	5.872	5.776	5.711	5.750

Table-3.5 Intermolecular free length (L_f) at different temperatures of oils for 4MHz frequency

T (kelvien)	Intermolecular free length (Lf) :-$L_f = K_T\beta^{1/2}10^{-11}$ m			
	Palmolein oil	Groundnut oil	Mustard oil	Sunflower oil
303 K	4.676	4.591	4.569	4.592
308K	4.740	4.676	4.694	4.667
313 K	4.840	4.800	4.786	4.786
318 K	4.933	4.893	4.865	4.882

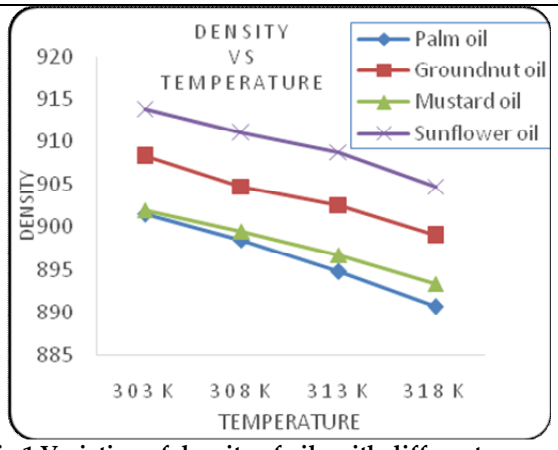

Fig.1 Variation of density of oils with different temperatures

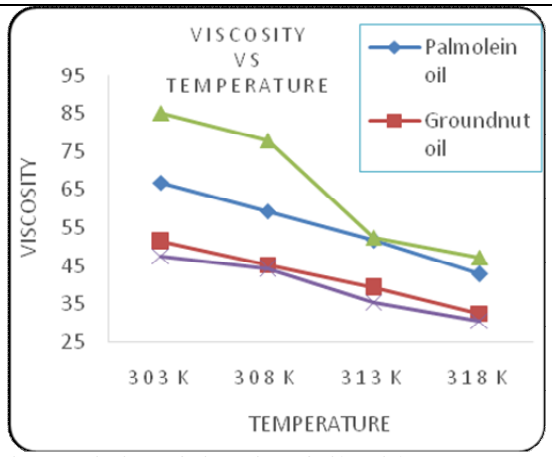

Fig.2 Variation of viscosity of oils with temperatures

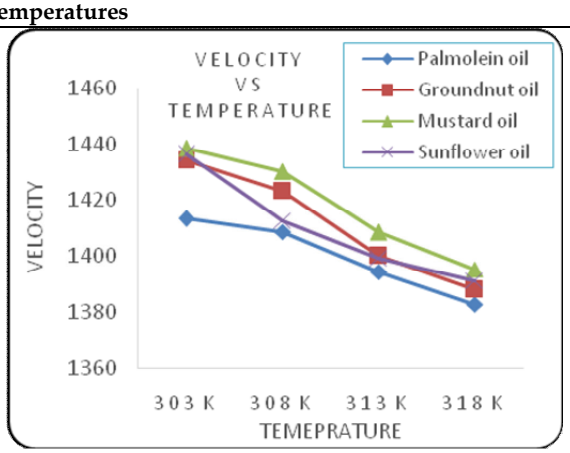

Fig. 3Variation of velocity of oils with temperatures

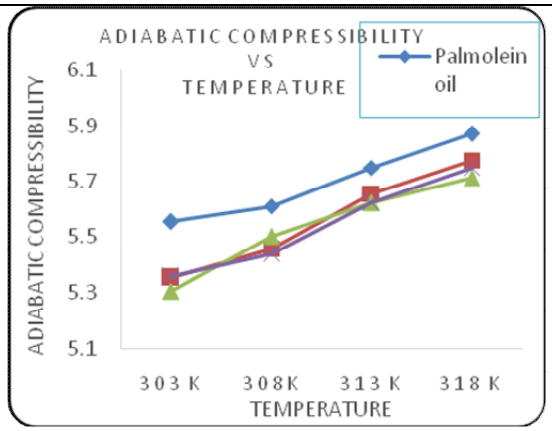

Fig. 4 Variation of adiabatic compressibility of oils with temperature

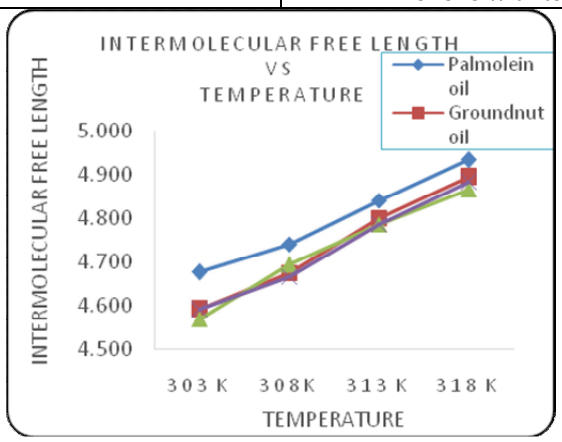

Fig. 5 Variation of Intermolecular free length of oils with temperature

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RESEARCH ARTICLE

Floral Waste Management by Offering Vermicomposting using Earthworm: *Eudrilus eugeniae*

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ABSTRACT

Production of huge organic wastes along with poor management system, results in a significant environmental degradation. The systematic and safe disposal is a major issue in number of cities of developing countries. In India at most of the religious places a huge amounts of s biodegradable waste are generated which contains fruits, flower, food waste etc. The quantity of flower waste in India is 300 MT/day. Odisha is considered as one of the holy state of India. Jatni is nearer to the temple city of Bhubaneswar. Large amounts of flowers are used during functions, worships, ceremonies and festivals. The quantity of floral waste generated by few major temples of the city was assessed for composting. In present study different proportions of soil, cattle dung and floral wastes were taken in form of mixture and performed vermicomposting process using earth worm species *Eudrilus eugeniae*. The study was designed with variation of these contents with different ratios. Soil with cattle dung was kept as control throughout the study. After Vermicomposting process analysis of various physical and chemical parameters was done. It was found that in almost all proportions the vermicompost was produced within a maintained parameters of temperature 23 degree Celsius, pH about 6.53 to 8.06 pH, 55% moisture content. Thus, vermicomposting of temple flower waste is an excellent and eco-friendly method to get valuable products which will lead to a healthier and waste free environment providing with an enriched manure for sustainable plant growth.

Keywords: Organic waste, floral waste, Vermicomposting (VC), *Eudrilus eugeniae*

INTRODUCTION

In present day all corners of the world is managing different organic wastes at low capital and operation cost as well as in eco-friendly and energy saving has attracted much attention. The cities and towns of India like other developing countries also suffer with solid waste management(Kaur and Joshi 2002). Vermicomposting of flower waste not only prevent damages to natural sources but help to some extent, in cleaning the nature.Huge amounts of flowers are offered in temples of Jatni city, Khurda, India creating a large amount of flower waste, which creates severe environmental pollution and health hazards. These materials are wholly biodegradable. Reduce, recycle and reuse of the organic waste is big challenges for municipal authorities in developing countries. The generation of waste is increasing in faster rate due to urbanization, industrialization, rapid expansion of cities and migration of people from rural area to urban area. To preserve the global agro-ecosystems and protect human health from the harmful agro-chemicals "Ecological Agriculture and Organic Farming" has to be promoted (Gomiero, 2008). Various biological management options offers for organic wastes instead of disposal to landfill sites, open dumping or any other environmentally risky waste management as alternatives, but vermicomposting is amost promising method for recycling. (Sangwan et al 2002, Aalok et al 2008, Adhikary et al 2012)

To convert floral waste into useful organic fertilizer would be of great benefit by using biological processes such as composting followed by vermicomposting. In this process the combined action of earthworms and microorganisms produce stabilized products as organic manure after transforming energy rich and complex organic substances (Edward et al 1992).Earthworms play a considerable role by fragmenting and altering all biological activity of the waste (Dominguez, 2004). Ecological agriculture is relatively more sustainable, and it could be an economically and environmentally viable alternative to the destructive chemical agriculture. According to many religious beliefs, flowers that are offered during prayers are sacrosanct and cannot be dumped into the garbage once they've wilted. This is one of the reasons why people prefer to discard them in rivers, lakes and other water bodies. But not many of us think about the fertilizers and pesticides that might have been used to grow these flowers, which then mix with the water and pollute it. These materials are wholly biodegradable which can be utilised effectively a "biological fertilisers'' for vegetables crops will not only provide economic benefits to the farmers but also improves and maintain soil fertility and sustainability in natural soil eco-systems (Kannaiyan, 2002). Thus, the prime objective of the of this study is to produce organic manure for establishing a sustainable plant growth by adding live earthworms (*Eudrilus eugeniae*) in the pots using various proportion of wastes to establish vermicomposting (Kinberg,1867). The recycling technology of biological method such as vermicomposting use for flower waste not only provide nutritional value to soil but also aid to cleaning environment.

MATERIALS AND METHOD

Collection of Materials

- Flower waste which are left unused after offering was collected from various temples nearby Jatni,Odisha,India.
- Fresh cattle dung and soil were collected in plastic bags from dairy farm at CUTM campus, Jatni, Odisha, India

Segregation of non-biodegradable substances

Manual segregation of flower waste was carried to remove the debris (plastic, threads, incense sticks, coconuts etc). The garlands and flowers were segregated and shredded into small pieces .to collect biodegradable waste

Pre-composting

The segregated floral waste was mixed with cattle dung with appropriate proportion (3:2) were allowed to decompose for seven days for semi-decomposition and stabilization to have optimum action of earthworm and

suitable for the process of vermicomposting because its thermophilic nature helps in mass reduction and pathogen reduction (Nair et al., 2006)

Collection and selection of earthworm species

The earthworm (EW) species *Eudrilus eugeniae* was collected from the vermicomposting unit of CUTM Campus and kept in a separate controlled environment before experiment. The species has potency to survive in different moisture content and resistance for temperature.

Drying and sieving of sample

For the growth of earthworms, the primary essential collected materials such as soil and cow dung were allowed to dry for a week spreading over plastic sheets. The air dried materials were sieved by a sieve of 36 nm and collected in a plastic bags.

Preparation of vermin bed

The process of vermicomposting was started by making portable vermi-bed using six plastic containers of length (l) 40 cm, breadth (b) 28cm and height (h) 12cm brought from market and labelled as control(C), P1, P2, P3, P4 and experimental (E) respectively.

Preparation of vermicomposting

The vermicomposting for floral waste was made in small scale. The dried material such as soil and cattle dung including pre composting floral waste were weighed in the help of weighing machine for various proportions. The experimental design was carried out by making 1:1 proportion of soil and cattle dung for each container except experimental which contained 100% of pre composting floral waste. The P1,P2,P3 and P4 were added with various proportion of 20%,40%,60% and 80% of pre composting floral waste to previous contained 1:1 proportion whereas control(C) only dealt with 1:1 soil and cattle dung proportion. The adding material were well mixed and allowed for making vermi-bed by forming layers. Two layers of floral waste and mixture of soil and cattle dung were placed over one another alternately. The earthworm *Eudrilus eugeniae*were measured with their length (l), perimeter (p) and diameter (d)ranging from 7.7cm to 13 cm and allowed to introduce four in number into vermi-bed of each container by adding slurry of cattle dung at top of the bed. After adding the earthworms were moved down and the sets were monitored throughout the period of vermicomposting by sprinkling of water to maintain moisture content and adding of slurry within a time interval of 4 days upto 45-50days. Monitoring of the process from every aspects was carried out upto 60-65 days where the entire mixture of the containers ready for harvesting vermicasts the black granular materials with a range of 0.7cm to 1cm. The physical parameters such as electro-conductivity, pH, moisture content of mixture, growth and survival of earthworm were estimated before and after vermicomposting, The growth and survival rate was measured with a time interval of fifteen days during entire period of vermicomposting that mentioned in tables and graphs. The population of the earthworm was measured by counting manually in each proportion within time interval of fifteen days also represented in tables and graphs.

RESULT AND DISCUSSION

The experiment on vermicomposting using floral waste was presented with number of tables and plotted graph contain the estimated values of different parameters. The present work is conducted to manage and utilize the floral waste generated by temples of Jatni city. The process of composting was carried out in different ratios of waste,soil and cow dung for 60 days. Earthworm species *Eudrilus eugeniae* was shown the activity of vermicompost because of it's adaptability to varied conditions on different proportion C(control),P1,P2,P3,P4 and E(experimental). The Table.1 was shown increase in the pH values of each container after vermicomposting in a range of 6.36-7.00 whereas the pH of experimental reached to a range from 6.67 to 8.06 indicated the formation of soil nutrient with decreasing of the toxicity floral waste. Graph-.1 was plotted with the physical parameters pH and temperature. The Table.2 was shown

the huge change in electro-conductivity of each proportion which indicate the salinity content of mixture converted during vermicomposting is applicable for agriculture requirement range especially in P3 and P4 proportion. The electro-conductivity of experimental as well the control value was significantly converted from its initial value indicated the increase of nitrogen content along with salinity as it mixed with cattle dung earlier. Graph.2 was presented the value of electro-conductivity of each proportions.Table.3 was shown the moisture content of each proportion was converted to the range of agricultural soil (75-95 in percentage).The moisture content was in descending order from control to experimental plotted in graph indicated that all proportion reached to a range of agricultural aspects especially in P3 and the experimental shown low content of moisture. The Graph.3 was shown the moisture content of all proportions. The growth of the earthworm during vermicomposting was estimated in Table.4 by measuring the length and diameter of the introduced earthworms filtering from the growing population. The difference of the initial and final value of l and d was calculated and plotted in graph which indicated the growth of earthworm increases in almost all proportion and more significantly in P3 whereas in experimental it was shown less growth due to increase in all parameters plotted on Graph.4.In Table.5 it was presented the number of earthworm was produced during vermicomposting after only introduced 4 in number before the process has been carried out. The number of population has been increased subsequently in P3 as compared to other but still in other proportions the production of earthworm was favoured was presented in Graph. 5. The organic manure was obtained with black in all proportion whereas found brown colour in P2 and P3.

DISCUSSION

The above results were explained that all parameters favourable towards suitable vermicompost that was obtained from P3 proportion as compared to other. But in other proportions the parameters also gave a significant role for different parameters like electro-conductivity,pH, moisture and growth of earthworm *Eudrilus eugeniae* during vermicomposting. In the present study it was found that the population of earthworm subsequently increased in all containers but the result of P3 is more effective as it was obtained with all suitable parameters presented in Table.5 and Graph.5. The quantity of vermicasts of all container was reciprocal obvious to population of earthworm

CONCLUSION

The results obtained from the present study was estimated the population rate of *Eudrilus eugeniae* more effective during vermicomposting of flower waste amended with proportion of cattle manure. The population of earthworm was produced the enriched end product vermicasts with high carbon nitrogen profile as confirmed through different parameters. The population of earthworm in the process of vermiculture was suitable for all adverse conditions. In the present work the result was produced more significantly in the mixture of low amount of soil and cattle dung mixture with high percent of flower waste of P3 proportion. The rate of population growth was indicated the amendment of floral waste due to the action earthworm. It helped to reduce the volume of agro waste additional to produce eco-friendly and cost effective manure for agricultural application. The present work can be established in large scale in future to obtained organic floral manure as well as the vermiculture of *Eudrilus eugeniae* for amendment of other solid waste.

REFERENCES

1. Aalok, A., Tripathi, A.K., Soni, P., 2008. Vermicomposting: A Better Option for Organic Solid Waste Management. J. Hum. Ecol. 24 (1), 59-64.
2. Adhikary, S. 2012. Vermicompost, the story of organic gold: A review. Agricultural Sciences, 3,905-917 doi:10.4236/as.2012.37110.

3. Edwards, C.A., Bater, J.E. 1992. The Use of Earthworms in Environmental Management. Soil Biol. Biochem. 24 (12), 1683–1689.
4. Gomiero,T.,Paoletti,M.G., and Pimentel,D.2008. Agricultural "wastes" for cellulosic ethanol production: a beneficial option or a real threat? In preparation.
5. Gomiero, T., Giampietro, M., and Mayumi, K. 2006. Facing complexity on agro-ecosystems: a new approach to farming system analysis. Int. J. of Agric. Res.,Gov. and Ecol. 5: 116–144
6. Gomiero, T., Giampietro, M., and Mayumi, K. 2006. Facing complexity on agro-ecosystems: a new approach to farming system analysis. Int. J. of Agric. Res.,Gov. and Ecol. 5: 116–144
7. Gomiero, T., Giampietro, M., and Mayumi, K. 2006. Facing complexity on agro-ecosystems: a new approach to farming system analysis. Int. J. of Agric. Res., Gov. and Ecol. 5: 116–144
8. Kannaiyan, S. (2002) 'Role of biological fertilizers, biopesticides, and their quality control in vegetable production', Proceedings of International Conference on Vegetables, 11–14 November, Bangalore, India, pp.461–489.
9. Kaur, S., Joshi, N. 2002. Solid Waste Generation During Normal Days in Haridwar City. Him. J. Environ. Zool.16 (2), 267-270.
10. KinbergJGH.(1867) Annulatanova. ÖfversigtafKöniglichVetenskapsakademiensförhandlingar, Stockholm 23 (9):337-357 [poiop[][pol;
11. Nagavallemma, K.P., Wani, S.P., Stephane, L., Padmaja, V.V., Vineela, C., Babu Rao, M. and Sahrawat, K.L. (2004) 'Vermicomposting recycling wastes into valuable organic fertilizer', International Crops Research Institute for the Semi-Arid Tropics Report, No. 8, p.20
12. Nair, J. ,Sekiozoic, V., Anda, M., 2006. Effect of pre-composting on vermicomposting of kitchen waste ,J Bio resource Technology, 97 2091–2095
13. Sangwan, P., Kaushik, C.P., Garg V.K., 2002. Vermicomposting of sugar industry waste (press mud) mixed with cow dung employing an epigeic earthworm Eiseniafoetida. Wast. Manag. Res. 28(1):71-75.
14. Singh, A., Jain, A., Sharma, B., Abhilash, P., Singh, H.: Solid waste management of temple floral offerings by vermicomposting using *Eiseniafetida*. Waste Manag. **33**, 1113–1118 (2013)
15. Sinha, R.K. (1998) 'Embarking on the second Green Revolution for sustainable agriculture in India: a judicious mix of traditional wisdom and modern knowledge in ecological farming', Journal of Agricultural and Environmental Ethics, Vol. 10, pp.183–197
16. Gomiero, T., Paoletti, M. G., and Pimentel, D. 2008. Agricultural "wastes" for cellulosic ethanol production: a beneficial option or a real treat? In preparation
17. Guthman, J. 2004. Agrarian Dreams: The Paradox of Organic

Table.1(Measurement of physical parameter pH and temperature of vermicompost)

No of Reading	Name of Containers	Initial of pH	Final of pH	Temperature before vermicompost	Temperature after vermicompost
1	Control	6.78	6.89	23.4° C	26°C
2	P1	6.53	6.65	23.3°C	26°C
3	P2	6.36	6.45	23.2°C	26.2°C
4	P3	6.81	7.00	23.3°C	26.5°C
5	P4	7.07	6.88	23.2°C	27°C
6	Experimental	8.06	7.86	23.3°C	29°C

Table.2 (Measurement of physical parameter electro-conductivity of vermicompost)

No of readings	Name of Pots	Initial readingof electro-Conductivity	Range In µ	Final reading of electro-Conductivity	Range In m
1	Control	115.1	200	1.293	2
2	P1	85.4	200	1.165	2
3	P2	44.5	200	1.265	2
4	P3	100.3	200	0.691	2
5	P4	44.8	200	0.478	2
6	Experimental	96.5	200	1.359	2

Table.3 (Measurement of moisture content of vermicompost)

No. Of Readings	Name of Containers	Weight of Wet Compost Soil	Weight of Dry compost Soil	Difference(moisture content)
1	Control	2gm	1.1363gm	0.8637gm
2	P1	2gm	1.0694gm	0.9706gm
3	P2	2gm	0.9391gm	1.0609gm
4	P3	2gm	0.8539gm	1.1461gm
5	P4	2gm	0.7914gm	1.2086gm
6	Experimental	2gm	0.639gm	1.361gm

Table.4 (Measurement of growth through length and perimeter of Earthworm)

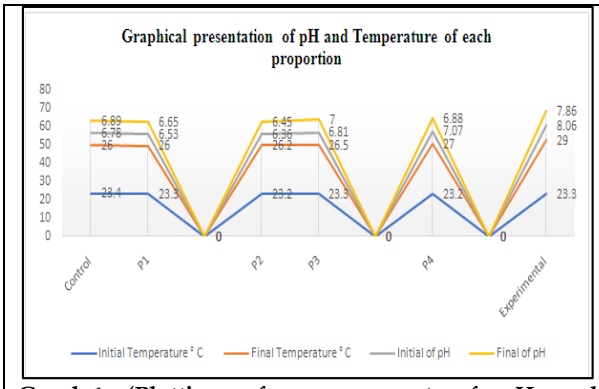
(Measurement of Earthworms before and After Introduce)

Name of Containers	Initial Length (l) of EW before VC in cm	Final Length (l) of EW after VC in cm	Diff. In Length (l)	Mean	SD	Initial Perimeter(p) of EW before	Final Perimeter(p) of EW after	Difference in diameter (p)	Mean	SD
Control	13	14.2	1.2	0.95	0.26	1.3	1.5	0.2		
	9.9	10.8	0.9			1.4	1.6	0.2		
	12.8	13.6	0.6			1.3	1.4	0.1	0.17	0.05
	9.7	10.8	1.1			0.9	1.1	0.2		
P1	11.7	12.4	0.7	0.72	0.05	1.2	1.5	0.3		
	11.8	12.6	0.8			0.9	1.1	0.2		
	12.2	12.9	0.7			0.8	1	0.2	0.22	0.05
	9.8	10.5	0.7			1.3	1.5	0.2		
P2	12.9	10.5 13.2	1.4	0.75	0.46	1	1.2	0.2		
	12.6	13.3	0.3			1.7	1.9	0.2	0.2	0.08
	11.3	11.9	0.7			1	0.8	0.2		
	11.6	12.6	0.6			1.2	1.4	0.2		
P3	12.9	13.2	1.2	1.175	0.21	1.5	1.7	0.2		

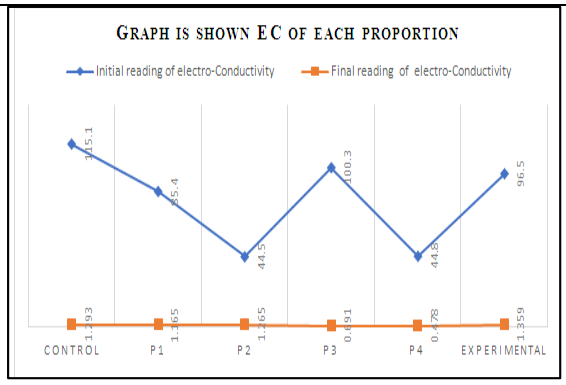
	12	13.2	1.2			1.3	1.6	0.3		
	12.2	13.3	1.2			1.4	1.5	0.1	0.22	0.09
	11.9	12.8	0.9			1.4	1.6	0.2		
P4	9.7	10.5	0.8	0.925	0.34	1	1.2	0.2		
	9.7	10.9	1.2			1.1	1.4	0.3		
	11.3	12.6	1.3			0.9	1.1	0.2	0.25	0.05
	10.7	11.2	0.5			1.2	1.3	0.1		
Experimental	12.5	13	0.5	0.725	0.04	1.5	1.6	0.1		
	11.2	11.9	0.7			1	1.2	0.2	0.175	0.05
	9.9	10.3	0.4			1.2	1.4	0.2		
	9.8	11.1	1.3			1.1	1.3	0.2		

Table.5 (Population growth of earthworm during vermicomposting)

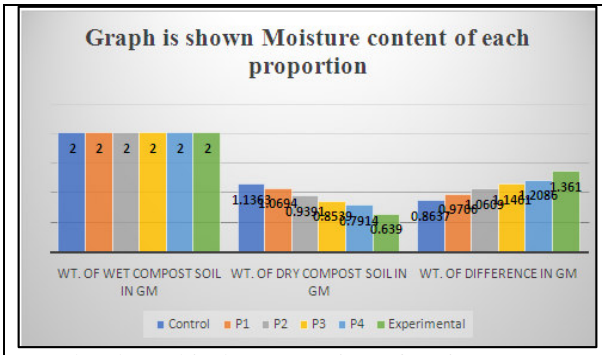
Name of Containers	Initial population of EW before VC	Final Population of EW after VC(mean value)
Control	4	27
P1	4	22
P2	4	18
P3	4	36
P4	4	14
Experimental	4	16



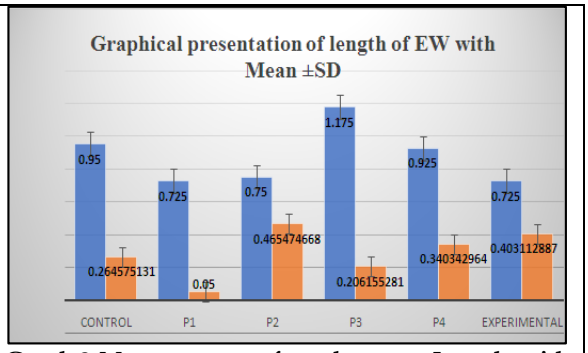
Graph.1 (Plotting of measurement of pH and temperature value of various Proportion)



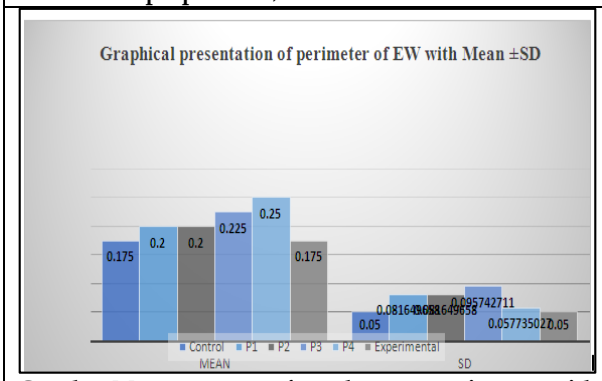
Graph.1.1 (Plotting of measurement of E.C of each Proportion)



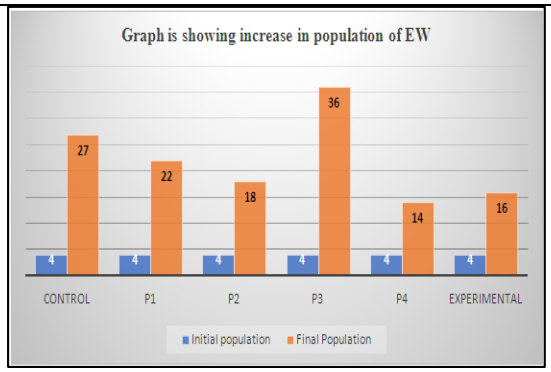
Graph.2 (Graphical presentation of moisture content of different proportions)



Graph.3-Measurement of earthworms Length with respect to Mean ±SD



Graph.4-Measurement of earthworm perimeter with respect to Mean ±SD



Graph.5 (Population growth of earthworm during vermicomposting)

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RESEARCH ARTICLE

Management of Industrial Waste Fly Ash through Vermicomposting by using *Eudrilus eugeniae*

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ABSTRACT

Generation of huge amount of various wastes are dumped the earth and considered serious environmental problems. A large amount of Fly Ash (FA) are one of them produced from coal based Thermal power plants for fulfilment of power generation which is now causing an acute global disposal problem. Hence Fly ash management remains a major concern for the world in the 21st century. Effective and safety disposal of these Fly Ash wastes is considered as a major recycling process through vermicomposting. Hence, vermicomposting is a cost-effective method being considered as sustainable economical solution in suitable management of fly ash. Fly ash management is an excellent method for reducing the toxic heavy metals by the combine action of earthworms and microbes to produce enriched product as vermicompost after minimize the solubility of heavy metals and increase the bioavailability of major nutrient elements. In the present work various proportion of coal based FA amended with mixture of soil and cattle dung at periodical intervals with introduction of a special earthworm *Eudrilus eugeniae.* The result is obtained with the successful conversion of FA into vermicompost in various ratio in respect to various concentration of FA with the changing physico-chemical parameters, population growth, and nutrient content during vermicomposting. Vermicomposting of flyash is stimulated the soils nutrient by microbial growth and activity of earthworm and enhance the fertility of the soil for sustainable agricultural production.

Keywords: Fly Ash (FA), vermicomposting, *Eudrilus eugeniae*

INTRODUCTION

Including India for most of the developing countries, the major focus area is electricity, the engine of growth generated form number power plants. The huge production electricity all over the world for fulfilment demand of rapid urbanization growth. A major source of electrical energy is coal-based thermal power plants (Mrityunjay,2017).Coal is abundantly available, and a major source of energy till date (Research gate, 2015). The annual generation of fly ash has been increased which is a fine, glass powder recovered from the gases of burning coal during the production of electricity or power generation. (Zeba Usmani, 2016). Fly ash (FA) is a resultant of coal and lignite combustion at thermal power plant having toxic heavy metals in it. FA is a waste material to pollute the environment considered as "Polluting Industrial Waste" due to very few utilization areas of fly ash were known hence the general perception of people about fly ash was negative (R.M Venkatesh,2008) Thus, in the present situation it is highly essential for proper utilization and management of FA.A great potentiality of FA for agriculture application and is quite economical to use as a soil amendment. FA contains essential plant nutrients like Ca, Mg, S, Si, Al, Fe, and Na that are beneficial for plant growth and has advantage of enhancing nutrient availability in the soil for better agriculture.

A promising and significant ways to recycle the industrial wastes generated from power plant is composting. The process in which wastes are converted into nutrient-rich organic manure known as vermicomposting where earthworms are used as the biological agent (Edwards &Bater 1992). It is an eco-friendly, cost effective and faster method of producing organic fertilizer from waste materials. The end product of this process is vermicompost contains water-soluble nutrients and is an excellent fertilizer and acts as a good soil conditioner. Vermicomposting Improvement in soil aeration, enriched soil with micro-organisms, microbial activity in worm castings is 10 to 20 times higher than in the soil and organic matter that the worm ingests, improves water holding capacity are carried out during and after vermicomposting (P.Saranraj). For the degradation of Fly Ash (FA) waste,it's mass reduction and recovery of nutrients through vermicomposting is played a great role by earthworms (Allan Mupambwa). Vermicomposting has emerged as an effective technique for mitigation of metals available in FA (Bhattacharya,2004). Fly ash based vermicomposting will help in bulk utilization of the fly ash which is a waste product and otherwise may also cause groundwater contamination. (V. Kumar, 2005) Earthworms are important sources and considered as natural bioreactors. These are like to be wet and need adequate moisture to help them breathe through their skin. Vermicomposting worms can convert waste materials into mineralized forms as vermicompost a nutrient-rich, biologically beneficial soil product(Adhikary,2012). It is the process in which earthworms remove toxins from the FA or FA mixture through bioaccumulation of heavy metals from coal ash or contaminated site/land. The heavy metals of the FA is ingested by earthworm convert them into valuable vermicompost while passing through it's gut and interacted with microbes that consumed. The combination of FA and organic amendment improves the microbial functions and further the efficiency of FA a source of plant nutrients in agriculture(Mohapatra&Rao 2001, George et al. 1998).

Earthworm, being a soil dwelling organism, feeds on soil, litter and other organic matter. They inevitably consumethe soil microbes during ingestion of litter and soil. Earthworm belongs to class Oligochaeta of phylum Annelida being a soil dwelling organism, feeds on soil, litter and other organic matter. They inevitably consume the soil microbes during ingestion of litter and soil. Earthworms may also enhance the fertility of soil treated with coal fly ash by increasing solubilisation of mineral nutrients. Vermicomposting is one of the recycling technologies, which improves the quality of products (Earthworm Ecology,1983). It involves using earthworms to increase the microbial population in vermicasts and help to produce high-quality compost from different organic wastes in a lesser period. Theaim of the present investigation was to produce vermicompost by using *Eudrillus eugeniae* concerning the various proportion of fly ash during vermicomposting with related to all suitable physico-chemical parameters. The combination of fly ash with soil and cattle dung is much beneficial during vermicomposting that will ensure sustainable management of bulk waste and environment.

MATERIALS AND METHODS

Preparation of Vermicomposting

Collection of Materials

Fly Ash (FA) is fined powder waste samples were collected from IB thermal power station,Jharsuguda, Odisha, India.Cattle dung (CD)and soil (S) were collected from Centurion University of Technology and Management (CUTM) campus, Bhubaneswar, Odisha,India, in order to expedite the bioconversion process.

Collection of Earthworm Species

Certain species of earthworm (EW) only essential for vermicomposting as per literature study. The earthworm species *Eudriluseugeniae*were collected from the vermiculture unit of the CUTM Campus. The species selected for vermicomposting is *Eudriluseugeniae* (Mature about 45–60 days old) healthy Clitellated species comprising a weight of about 250–320 mg were collected.

Drying,Sieving of Collected Materials

The collected cow dung and soil are exposed in bright sunlight for drying, then large size cow dungs are chopped into smaller pieces and allowed for further drying. After drying the soil and the cow dung were crushed in to tiny particles and the large and unwanted materials were separatedbysievingprocess through a sieve of diameter of 3.55 mm.

Experimental Set up for Vermicomposting

The vermicomposting process was carried out with experimental set up by using 6 plastic containers The 6 containers were labelled as control (C), Pr1,Pr2 ,Pr3, Pr4, and experimental (E). The 6 different proportions were formed for 6 labelled containers by using the 3 collected, sieved and dried materials such as soil, cow dung and Fly Ash (FA) as treatments follows:

1. C= Pure cattle dung + Soil (1:1) + *E. eugeniae*
2. Pr1=Cattle dung + Soil +Fly ash (1:1:2) + *E. eugeniae*
3. Pr2=Cattle dung +Soil +Fly Ash(1:1:4) + *E. eugeniae*
4. Pr3=Cattle dung +Soil +Fly Ash (1:1:6) + *E. eugeniae*
5. Pr4=Cattle dung + Soil + Fly ash (1:1:8) + *E. eugeniae*
6. E= 100% Fly Ash (FA) + *E. eugeniae*

Pr= Symbolised for Proportion and CD+S+FA forCattle dung + Soil +Fly ash

All the treatmentsof CD+S+FA were allowed for precomposting before inoculation of earthworm.

Preparation of Pre-composting

All the various proportions of FA withCattle dung + Soil were prepared having 1kg of mixture per each container by weighing through the help of weighing machine and mixed uniformly. Water was sprinkledinto all proportion for maintaining moisture contentin the mixture and allowed for composting about 10 days without adding earthworm in shady regions which later formed pre-compost.The treatments were left before the inoculation of earthworms for thermal stabilization, initiation of microbial degradation and softening of substrate material helps in mass reduction and pathogen reduction in the process of vermicomposting (Nair et al., 2006). Sample from all mixture were collected before and after adding water for physico-chemical analysis. (Pr= symbolised for proportion)

Preparation of Vermicomposting bed

The Preparation of vermicompost bed was performed in the laboratory in plastic container. The precomposting materials was removed from each container separately and applied as stacks of layers again in the respective

containers adding slurry in between these as bed. After preparation of vermicomposting bed 3 number of earthworms *Eudrillus eugeniae* (the nightcrawler) were inoculated in each container.

Method of Vermicomposting

The process of vermicomposting was carried out for 70-80 days till the formation of vermicompostwhich was monitored with respect to physical changes in mixture composition by regular growth, nutrition and different physico-chemical parameter of the earthworm. The physico-chemical parameters like pH, optimum temperature, electro-conductivity and moisture content of the treatments were maintained and recorded at an interval of 15 days (0, 15, 30, 45,60 days). The chemical analysis of Fly Ash and changes in mixture during vermicomposting were observed.

RESULT AND DISCUSSION

The present study on vermicomposting of various proportion of Fly Ash was obtained with different values of physico-chemical parameters,growth activity with survival rate of earthworm and the type of vermicompost and estimated through number of Tables and Graphs. The vermicomposting process was estimated with the activity of *Eudrilus eugeniae* that has adaptability to varied condition provided with the composting mixtures C (control), Pr1, Pr2, Pr3, Pr4 and E (experimental).The physico-chemical parameters pH, moisture content,temperature and electroconductivity were easily adopted by earthworm and carried out the formation of vermicomposting along with the action of supporting microbes. The growth in population of earthworm were significantly increased at a time interval of 15 days in all treated container with adding proper nutrition as slurry, indicator of the formation of vermicompost due to suitable conversion in physico-chemical parameters during the entire process of vermicomposting was shown in Table-1 and Graph-1.The muscular grinding organ gizzard of earthworm rapidly fragmented the waste into finer particle after consumption and releases dark black granular vermicast normally ,similar concept with (Lakshmi Prabha et al 2014).In this study it was observed that black granular vermicast resulted except Pr4 and FA (experimental) where it was released with greyish brown colour was shown in Table-2 and Graph-2. About 60% of whole FA was converted into vrmicompost in the container shown a slow dgradable process compared to other proportion.During the process of vermicomposting the earthworm are aerators that it emits sufficient oxygen to oxidize foul smell producing compounds to make odourless vermicompost (Nagavallemma et al , 2000)

The variables of electro-conductivity (EC) and pH were shown in Table-3and Graph-3 explained that in the initial stage of vermicomposting EC increased and became reduce later due to addition of nitrogen content with salinity.Similarly the pH is converted from slightly acidic to neutral while the whole FA converted towards neutral from alkalinity indicated reducing the toxicity of FA from various proportion. The microbial nitrification process of nitrifying bacteria present in wastes were cause of releasing volatilization of ammonical nitrogen and H+.(Singh,et al 2005, Eklind and Kirchmann ,2000)and increased the mineral salts initialy and later reduce to convert into insoluble salts (Nisha Jain,2016). The moisture content of each proportion was converted to the range of agricultural soil (upto75%) except in Pr4 and experimental was low due to compactness of FA, similarly the temperature in all proportion was maintained below 30^0C at final stage of vermicomposting was shown in Table-4 and Graph-4. In each of the ouput that discussed was progressed positively with the range of agriculture application for the treated container Pr2 and Pr3 as compared to other.

CONCLUSION

The heavy metal contained Fly Ash form the present study was observed that the waste along with addition of soil and cattle dung degraded slowly during vermicomposting technique carried out for 70-80 days by the action of

Eudrilus eugeniae. It can able to convert into *sustainable* agvricultural application by the action *of earthworm along with microbes* play animportant role to produce organic rich manure as vermicompost.The present study wasconcluded that *a* low percent of FAwith the mixture of cattle dung enhance the microbial activity to produce suitable vermicompost rapidly while increase in the percentage of FA in treated mixture require addition of water and slurry to improve the combine activity of earthworm and microbial action to accelerate the production of enriched plant nutrient vermicompost.

REFERENCES

1. Adriano, D. C., Page, A. L., Elseewi, A. A., Chang, A. C. and Straughan, I. (1980) Utilization and disposal of fly ash and other coal residues in terrestrial ecosystemsA review. J. Environ. Qual. 9: 333-334.
2. Adhikary, S. (2012) Vermicompost, the story o of organic gold: A review. Agricultural Sciences, 3,905-917 doi:10.4236/as.2012.37110.
3. Bhattacharya, S.S. andChattopadhyay, G.N. 2002. Bioavailability ofphosphorus from fly ash through vermicomposting. J. Environ.Qual.
4. Bhattacharya, S.S. and Chattopadhyay, G.N. 2002. Bioavailability of phosphorus from fly ash through vermicomposting. J. Environ. Qual., 31(6): 2116-2119.
5. Bhattacharya, S.S. and Chattopadhyay, G.N. 2004. Transformation of nitrogen during vermicomposting of fly ash. Waste Manage. Resour., 22: 488-491.
6. Bhattacharya, S.S. and Chattopadhyay, G.N. 2006. Effect of vermicomposting on the transformation of some trace elements in fly ash. Nutr. Cycl. Agroecosys., 75: 223-231.
7. Bhattacharyaa, S.S., Iftikar, W., Sahariaha, B. and Chattopadhyay, G.N. 2012. Vermicomposting converts ûy ash to enrich soil fertility and sustain crop growth in red and lateritic soils. Resour. Conserv. Recyc., 65: 100-106..
8. Edwards, C.A., Bater, J.E. 1992. The Use of Earthworms in Environmental Management. Soil Biol. Biochem. 24 (12), 1683–1689.
9. Gupta, S.K., Tewari, A., Srivastava, R., Murthy, R.C. and Chandra, S. 2005. Potential of Eiseniafetida for sustainable and efficient vermicomposting of fly ash. Water Air Pollut., 163(1/4): 293302.
10. Manivannan, S., Anbalagan, M. and Prakasam, B.A. 2012. Influence of earthworm Lampittomauritti (Kinberg) and organic additives for efficient vermicomposting of fly ash. Am-Eurasian J. Sci. Res., 7(2): 58-63.
11. M. C. Dash and B. K. Senapati, —Vermitechnology, an option for organic waste management in India,‖ in Verms and Vermicomposting, M. C. Dash, B. K Senapati, and P. C. Mishra, Eds., pp. 157–172, Sambalpur University, Sambalpur, Orissa, India, 1986.
12. *Lotzof, M. "Very Large Scale Vermiculture in Sludge Stabilisation".Vermitech Pty Limited. Retrieved 2012-10-03.*
13. Nagavallemma, K.P., Wani, S.P., Stephane, L., Padmaja, V.V., Vineela, C., BabuRao, M. and Sahrawat, K.L. (2004) 'Vermicomposting recycling wastes into valuable organic fertilizer', International Crops Research Institute for the Semi-Arid Tropics Report, No. 8, p.20
14. Nair, J. ,Sekiozoic, V., Anda, M., 2006. Effect of pre-composting on vermicomposting of kitchen waste ,J Bio resource Technology, 97 2091–2095
15. Singh, L.P. and Siddiqui, Z.A. 2003. Effects of fly ash and Helminthosporiumoryzae on growth and yield of three cultivators of rice. Bioresour. Technol., 86: 73-78. Singh, S.N., Kulshreshtha, K. and Ahmad, K. J. 1997. Impact of fly ash soil amendment on seed germination, seedling growth and metal composition of Viciafaba L. Ecol. Eng., 9: 203-208.
16. Adhikary, S. (n.d.). Retrieved from scientific research: https://www.scirp.org/html/4-3000330_24396.htm
17. Allan Mupambwa, A. l. (n.d.). Retrieved from www.sciencedirect.com: https: //www. sciencedirect. com/science/article/pii/S0956053X15301501
18. Bhattacharya, S.S. andChattopadhyay, G.N. 2002. Bioavailability ofphosphorus from fly ash through vermicomposting.

19. Mritunjaya, S. K. (n.d.). publishing. Retrieved from https:// pubs.rsc.org /en/content/ article landing /2017/ra/c6ra27329 g#!divAbstract
20. P.Saranraj. (n.d.). Retrieved from https://www.researchgate.net: https:// www.researchgate.net /publication/259495486_Vermicomposting and its importance in improvement of soil nutrients and agricultural crops
21. R.M.Venkatesh. (2008). Mass reduction and recovery of nutrients through vermicomposting of fly ash. Applied Ecology and Environmental Research,.
22. V. Kumar, G. S. (2005). Fly ash Utilization Programme (FAUP) TIFAC ,,. New delhi.
23. ZebaUsmani. (n.d.). publishing. Retrieved from https:// pubs.rsc.org/en /content/articlelanding /2017/ra/c6ra27329g#!divAbstract

Table 1. The population growth indicates survival of EW during vermicomposting

Sl. No.	Observations	Initial number of earthworm	Survival of earthworm in 1st 15days	Survival in 2nd 15days/after 1 month	Survival in 3rd 15days	Survival in 4th 15days	Survival in 5th 15days
1.	Control	3	3	6	12	17	24
2.	Pr-1	3	3	6	11	14	22
3.	Pr-2	3	4	13	19	26	31
4.	Pr-3	3	3	7	13	23	27
5.	Pr-4	3	2	4	3	7	11
6.	Experi-mental	3	2	3	3	6	10

Table 2.Colour and odour of vermicompost in all proportions after completion of vermicomposting

Sl. No.	Observations	Colour of vermicompost	Odour of vermicompost
1	Control	Dark brown	Odourless
2	Pr1	Black	Odourless
3	Pr2	Dark Black	Odourless
4	Pr3	Dark Black	Odourless
5	Pr4	Greyish Black	Odourless
6	Experimental	Greyish Black	Odourless

Table 3. Electro-conductivity and pH of fly ash proportions in vermicomposting

Observation	Sample in proportion	Electro-conductivity in S/m			pH		
		Initial	Final	Difference	Initial	Final	Difference
Control-100%	**OM (100%)**	114.9	152.3	37.4	6.48	6.62	0.14
Pr-3	**FA+OM(3:2)**	085.6	074.1	11.5	6.61	6.72	0.11
Pr-4	**FA+OM(4:1)**	126.9	103.8	23.1	6.72	6.84	0.12
Expt.(FA))	**FA (100%)**	096.4	070.4	26.00	8.01	7.34	0.67

Table 4.Moisture content and Temperature of fly ash proportions in vermicomposting

Observation	Sample in proportion	Moisture content						Temperature	
		During Precomposting			During Vermicomposting			Initiation of vermi composting	Completion of vermin composting
		Wet weight (in gm) Initial	Dry weight (in gm) Final	Difference	Wet weight (in gm) Initial	Dry weight (in gm) Final	Difference	Initial Temp. in ^{0}C	Final Temp in ^{0}C
Control-100%	OM (100%)	2.033	1.017	1.016	1.997	1.011	0.986	35	29
P-1	FA+OM (1:4)	2.023	1.031	0.991	1.983	1.021	0.962	35.5	26.2
P-2	FA+OM (2:3)	2.012	1.087	0.924	1.982	1.086	0.896	32.6	23.2
P-3	FA+OM (3:2)	2.023	1.078	0.944	1.998	1.072	0.926	31.4	23.9
P-4	FA+OM (4:1)	2.015	1.023	0.992	1.984	1.016	0.968	34	27.1
Expt.(FA)	FA (100%)	2.008	1.310	0.697	1.887	1.203	0.684	36	28.3

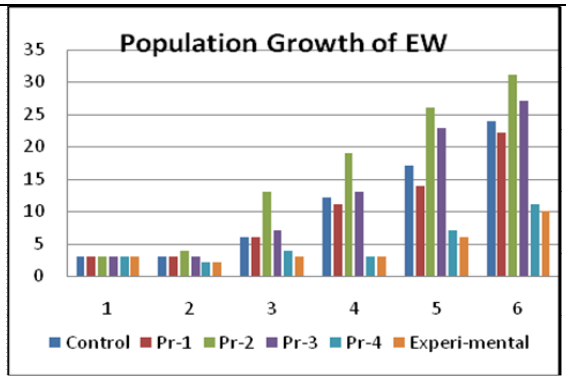

Fig.1 Graphical presentatio of Population growth of EW at the interval of 15 daysable

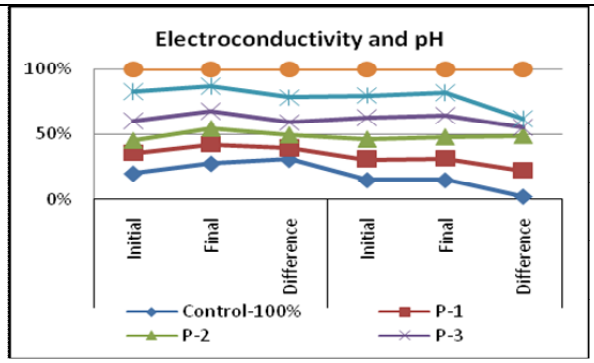

Fig.2Graphical presentation of EC and pH of FA proportions during vermicomposting

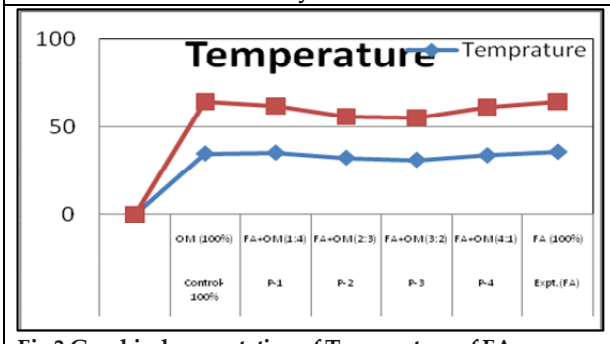

Fig.3 Graphical presentation of Temperature of FA proportions during vermicomposting

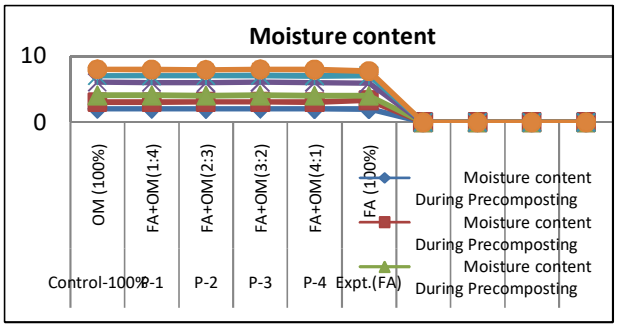

Fig.4 Graphical Presentation of Moisture content of all treatments during before and after Vermicomposting

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RESEARCH ARTICLE

Influence of Microbial Activity on Plant Growth Obtained from Vermicomposting Soil

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ABSTRACT

ABiological organic waste decomposition process yields the biofertilizer namely the vermicompost. The vermicompost is a result of combine action of earthworms and microbes through the process vermicomposting. It is an eco-friendly, cost effective, low technological composting process. The vermicompost produced as a result of vermicomposting process shows positive impact on plant growth rate, yielding capacity and health. To investigate the effect of vermicomposting bacteria on plant growth rate the present study was established by taking 4 pots labelled as T1, T2, T3, T4. Composting soils were taken in T1, T2, T4 while vermicomposting soil in T3. Bacteria from vermicomposting soil was cultured in nutrient broth, sprinkled on T2 for determining growth of Green gram plants and only nutrient broth was sprinkled on T4. All the parameters for growth is significantly favoured to treatment T2 as comparison with other treatments including control.It was observed from the study that the root length, shoot length, no. of root hairs, no. of branches, leaves, flowers and no. of pods per Green gram was more in T2 as compared to T1, T4 and the growth rate was almost equal to T3.

Keywords: Eco-friendly, Vermicomposting, Nutrient broth, Green gram

INTRODUCTION

Vermicomposting in which earthworms are for composting purpose along with the action of microorganism is a non thermophilic biological oxidation process converts the waste materials in to peat like material. The obtained material is vermicompost with good porosity, aeration, proper drainage, high water holding capacity and microbial activity (Edwards1998; Atiyeh et al2000b; Arancon et al2004a).Most cost effective and best waste management can be done

by vermicomposting process (Banu et al 2001; Asha et al 2008). Earthworms not only increase the microbial activity and degradation potency butalso drivers the aeration , conditioning and fragmentation process (Fracchia et al,2006; Lazcano et al,2008).The best alternative of conventional compost i.e. , the vermicompost biodegrade the organic wastes like medical waste, kitchen waste, crop residues, industrial wastes in to smaller fragments by the action of several enzymes, intestinal mucus and antibiotics present in Earthworm's intestinal tract(Gandhi et al,1997). In the non thermophilic decomposition process 2 to 5 times decomposition process speeds up the conversation of wastes into valuable homogeneous biofertilizer than thermophilic process (Bhatnagar and Palta1996;Atiyeh et al,200a).A wide range of difference in microbial activity and community between vermicompost and compost is found (Sublet et al,1998). In thermophilic composting process during active phase action of thermophilic bacteria is seen which is followed by mesophilic maturation phase (Lazcano et al, 2008; Vivas et al, 2009). The mesophilic process of vermicomposting mainly done by the action of mesophilic fungi and bacteria (Benitez et al, 1997). Combine action of microbes and earthworms is shown in active stage of vermicomposting while in maturation stage only the action of associated microbes is found. The maturation phase occurs only after the movement of worms to the fresh layer of undigested wastes. Species and density of earthworm is a major determining factor during the active decomposition phase (Ndegwa et al, 2000; Lazcano et al, 2008; Aira et al, 2011).

Various kinds of wastes such as horticultural wastes (Edwards,1998), mushroom wastes (Edwards 1998;Tajbaksh et al,2008), fecal matter of pig(Chan and Griffiths, 1998; Reh,1992), wastes from agricultural field (Bansal and kapoor 2000), cattle dung (Gandhi et al,2002), industrial effluents such as paper(Butt 1993; Elvira et al,1995;Gajalakshmi et al2002), sludge from diary plants and farms, paper mills (Elvira et al 1997;Banu et al 2001), refuses from kitchen ,hotels and hostels (Sinha et al 2002),animal and plant remaining and urban wastes(Edwards et al,1985; Edwards 1988) can be used in vermicomposting purpose (Sharma et al,2005). Gizzard of Earthworm converts the waste materials into various smaller forms which are released in the form of cast then gut microbes of Earthworm converts them to mature compost by action of various enzymes which is further known vermicompost (Dominguez and Edwards, 2004). Earthworm the segmented terrestrial inveterate worm is under the phylum Annelida. These creepy creatures have tube like or cylindrical, reddish brown segmented body having bilateral symmetry. A thick gilesteing delicate cuticle covers all over the body of the worm. Anterior side contains dark blood vessels while ventral surface represents genital opening. Clitellum present in the 14th and 16th segment helps to distinguish the anterior part i.e. mouth and posterior part i.e. the end.

On the basis of ecological habitat and functions Earthworm have following classified species i.eepgeic, endogeic and anecic (Brown, 1995; Bhatnagar and Palta, 1996).Small sized, uniformly pigmented Earthworms are epgeic species which have short life span and high reproductive rate. These worms are phytophagous in nature and normally eat surface litter. With the help of their active gizzard, they biodegrade the waste materials easily which speeds up the decomposition process. Besides the efficient biodegradation property they can also tolerate a high level of disturbances and releases large amount of nutrients. Epgeic species worms are *E. foetida,L . rubellus,L. castaneus,L. festivus,E. tetraedra ,Bimastusminusculus*. Endogeic specie worms are large weakly pigmented body .These geophagic worms can tolerate a medium range of disturbances and also have comparatively low life span than the epigeic specie. Endogeic species have ability to utilize the energy from poor soil, so these are used in soil improvement purpose .*Aporectodeacaliginosa, A. trapezoides, A. rose a ,Millsoniaanomala, Pontoscolexcorethrus* are some examples of endogeic specie . Endogeic specie is again divided in to followings such as polyhumicendogeic (small size body, surface dweller and feed on soil), mesohumicendogeic (medium size and feed on bulk soil), oligohumicendogeic (large size, feed on deep soil). Aneceics are large sized dorsally pigmented worm having low reproduction rate .These phytophageic, nocturnal earthworms are very sensitive to disturbances and made permanent burrows to live .*L.terrestrius, L. ployphemus* and *A. longa* belongs to the anecic specie (kooch and Jalilvand, 2008).*E. foetida* (Hartenstein at al, 1979),*E. Eugenie* (KaleandBano, 1988), *Perionyxexcavates* (Sinha et al, 2002; Suthar and Singh, 2008) are epigeic specie that are used in vermicomposting process. *Lampitomauritii* is a excellent compost producer (Ismail, 1997).
Earthworms, the bioengineers loosen the soil and increase the porosity of soil. The porous soil helps in easy penetration of root of plant and increases the water holding capacity, aerationproperty, microbial activity, and the

microbes present take active role in soil reclamation process (Nakamura 1996). Earthworm changes the physical, chemicaland biological property of soil and increases the productive rate of soil, so these are known as ecosystem engineer (Brown et al, 200; Munnoli et al, 2010) .Together action of microbes and earthworms causes decomposition and breakdown of large waste matters into smaller forms (Maboeta and Reneburg 2003).

Humidification mineralization makes the wastes to nutrient forms which are utilized by the plants (Lu, 1985; Ed wards and Bohlen 1996; chaioui et al; 2003). Earthworms are the drivers of important microbial activities (Edwards; 2004). Earthworms and micro organisms provide congenital conditions for the activities of microbes and also after biological activity of waste materials (Aira et al 2002). Earthworms cause change in chemical process of soil by increasing the microbial activity to decompose the waste material (Petersen and Luxton 1982; Lee 1985; Edwards and Bohlen 1996).Micro organisms and earth togetherily called ecosystem engineers (Lavelle; 1998). A large diversity of micro organisms are found in soil (Torsvik el al ; 2002).A large no of earthworm species utilize the soil bacteria (Pedersen and Hendrickson 1993) and soil fungi(Cooke and Luxton 1980; Edwards and Bohlen 1996).The microflora in the gut of earthworm depends upon various factors such as species of earthworm to be studied, feeding nature of worms, season (Kristufek et al. 1992).The no of microorganisms present in the earthworm's gut is determined by the feeding regime of the earthworm (Parthasarathi et al. 2007).

The microbial population presents on vermicompost causes various physico-chemical changes in the vermicompost by grinding and digesting the wastes which makes the vermicompost best biofertilizer (Maboeta and Van Rensburg 2003). Among all the microorganisms changes in bacterial community plays a major role during vermicomposting (Yasir et al. 2009).The bacteria isolated from vermicasts and earthworm's skin are mainly endospore forming gram Bacilli (Munnoli 2007). Various soil bacteria like *Bacillus ,Pseudomonas, Rhizobium and streptomyces* produces various metabolites which reduces the harmful microbes and pathogenic bacteria (Pathma et al.2011b).Micro and macro nutrients and microbial enzymes are present in huge amount in worm cast(Lavelle and Martin 1992).

MATERIAL AND METHODOLOGY

Study Area

The experiment was performed in the laboratory of Department of Zoology, Centurion University of Technology and Management, Jatni, Odish , India. The experiment was started on 1st week of November 2019 and ended on February 2020.

Sample Collection

About 2kg of composting and vermicomposting soil samples were collected in plastic bag from the Garden of Centurion University of Technology and Management, Jatni, Odisha, India.

Sample Preparation

Onegram of each soil sample i.e., composting and vermicomposting was taken after weighing in weighing machine. Then 1 gram of soil samples were taken in two clean and dry breakers each and then 9 ml of distilled water was added to the beakers to make 10 ml of solutions of each. The 2 beakers were then shaken properly for 10 minutes to get a proper agitation. After 10 minutes 1 ml of supernatant was taken from each beaker for serial dilution purpose.

Culture

About 0.1ml of each dilution was plated in nutrient agar medium underutilized condition and was incubated for growth. After 24 hours the plate count was carried out from each plate colony morphologyand stained each dominant colony byusing gram staining kit (Himediwpvt ltd). Again 0.1 ml of sample from 10 ml solution of vermicomposting soil was taken in cotton swab and incubated in nutrient broth for 24 hours at 33c temperature.After

24 hours 2 ml of nutrient broth (NB)and 2ml of bacterial cultured nutrientwere prepared for sprinkling on treated pots.

Experimental Application

Four pots were taken labelled as T1, T2, T3,T4where T3 contained with vermicomposting soil and rest 3 with composting soil. T1 was treated as control,T2was sprinkled with 2ml of cultured vermicomposting bacteria and T4 was sprinkled with only 2 ml of nutrient broth.All pots were sowed with soaked green gram seeds under aseptic condition.Germination of seeds were observed in all pots by regular monitoring of sprinkling water after adding of bacterial cultured in nutrient broth and nutrient broth. The observation of germination and growth in each pot was recorded at regular interval of 10 daysupto 2 months. In each 10 days interval the growing green gram tiny plants were pulled out from soil with proper care so that the root or any part not broken. Then the additional soil from the root was washed out and measured the root length. Shoot length and no of root hairs, no of flowers, no of pods no of branches and no of leaves were counted and recorded. For shoot length the measurement from base to the tip of the longest shoot was taken. Similarly base to of root to tip of the longest root represents the root length. Small hair like structures called root hairs were also calculated to find out bacterial effect on plant growth.

RESULT AND DISCUSSION

From the present experimentvarious morphologically different types of bacterial colony was obtained from composting and vermicomposting soil culturing shown in Table -2. The total CFU/ml in composting soil sample was $18x10^5$/ml and in vermicomposting sample was $27x10^5$/ml. The gram character of big white glassy colony (BWG) and small yellow glassy colony (SYG) was observed after staining.

Root Length

In all treatments it was shown an increase in length of green gram root. The root length in T_2 was all most equal that of T_3 but in T_1 and T_4 was no such rate of increase in root length. In T_2 the root length was 30.7cm and in T_3 it was 28.9cm after 60 days.

Shoot Length

The experiment was done to find out the activity of vermicomposting bacteria on plant growth when they were applied in composting soil. In T_1 and T_4 there was no such growth rate but the length of shoot was increased upto same length in T_3 and T_2such as 18.7cm and 19.5cm respectively.

Number of Root Hairs

The amount of root hair was also more in T3 and T2 as compared to T1 and T4. In T3 and T2 the number of root hairs was 93 and 97respectively.

Number of Leaves and Branches

It was observed from the above experiment that the vermicomposting bacteria put impact on plant growth when apply into normal composting soil. The T_3 and T_2 show more branches then T_4 and T_1. In T_3 and T_2 the no of branches was 10 and 12 respectively while T_1 had only 7 and T_4 had 8. Similarly, in case of leaves also T_3 and T_2 had more leaves i.e.30 and 36 respectively than T_1 and T_4 i.e. 21 and 27 respectively.

Number of Flowers and Pods

After application of vermicomposting bacteria to compost soil the number of flowers and pods were get increased in a significant manner and becomes similar as that in vermicomposting soil. After 90^{th} day of experiment the number of flowers in T_3 and T_2 was become 12 and 10 respectively and no. of pods per plant was 7 and 6 respectively. But in

case of T_1 and T_4 had the no. of flowers per plant was only 6 and 8 no of pods per plant was 3 and 4 respectively (presented Table-1). From the above experiment the growth rate is almost equal to the growth rate in vermicomposting.

DISCUSSION

The vermicompost was more enriched in nutrient for plant growth from every aspects as compared to natural oxidized composting soil . The PGPR bacteria in vermicompost increase the growth rate of plant by solubilizing the nutrients present in the compost (Ayyadurai et al 2007; Ravindra et al 2008 and pathma and sakthive, I 2012). As similar to our study the highest no of plant growth was seen in the soil treated with PGPR bacteria over control (R. Gopinathan and M. Prakash, 2014). In present study their occur a great change in bacterial colony number and character in composting soil as compared to normal composting soil (taken as control). Change in bacterial and fungal diversity in composting soil was observed previously (Insam et al 2009 et al 2005). There were also other studies which shows bacterial community changes during vermicomposting (Gopal, M. et al 2017; Cai et al 2018). A comparison study between vermicoposting and composting of sewage study and cattle manure was done by Lv et al (Lv et al 2015). As similar to our study Lv et al. and Huang et al. find out more no of bacterial diversity in vermicomposting the sample than composting one (Lv et al. 2015 ; Huang et al. 2013 . Huang and his colleges us had done their comparative analysis of no of bacterial diversity in 60 days old vermicomposting soil and also composting soil of same age. More amount of bacterial species richness and diversity was found in vermicompost of green waste than compost (cai et al. 2018). Our data provides a strong example of an increase in bacterial colony in vermicomposting soil as compares to compost. It was observed that the addition of nutrient and other organic matter activity of earthworm increases the amount of bacteria colony in vermicompost. Gupta et al observed a great increase in bacterial diversity in vermicompost of coconut and cow dung but after 75 days but the bacterial count decreasing moisture level (Gupta et al. 2017).\

CONCLUSION

Vermicomposting is a biochemical process in which the earthworms and associated microbes change the physico-chemical activity of the soil and waste matters and make them suitable biofertilizer.From the present investigationit was concluded that only presence of vermicomposting bacteria in composting or normal soil can give rise better yielding of plant as the same result found in vermicomposting. So we get to know that the microbes i.e. especially bacteria put a great impact in vermicomposting purpose along with earth worm. There is also found increase in the total CFU/ml in vermicompost as compared to compost. The above conclusion supports the work of Esakkiammal and LakshmiBai, 2013. They reported the increase in total no of bacteria and actinomycetes in earthworm gut than soil. In our experiment the seedlings of green gram with vermicomposting bacteria gives a better yielding as well as better plant growth. As our observation similar was done Prakash and Hemalantha in black gram in 2013 and found healthy seedlings. Finally the present study is focused with conclusion that application of only small amount of vermicomposting bacteria to normal compost soil can give better growth and yield than plants grown in only compost soil and the growth rate is all most equivalent with the growth rate of vermicomposting.

REFERENCES

1. Aira M, Gomez-Brandon M, Gonzalez-Porto, Dominguez J (2011) To study the selective reduction of pathogenic effect in cow manure in an industrial scale continuous feeding vermireactor. BioresourceTechnol (102) 9633-9637.
2. Arancon NQ, EdwardscA, Atiyeh R, Metzger JD. (2004a) Effect of vermicompost produced from food waste on growth rate and yield capacity of green house peppers .BioresourTechnol 93:139-144.

3. Asha A, Tripathi AK, Soni P (2008) Vermicomposting a better option for organic waste management. J Hum Ecol (24) 59-64.
4. Atiyeh RM, Dominguez J, Sublers, Edwards cA (2000a) To study the biochemical property of cow manure during processing by earthworm (Eiseniaandrei) and effect on seedling growth. Pedobiology(44) 709-724.
5. Atiyeh RM, Suble S, EdwardscA, Bachman G, Metzger JD, Shuster W (2000b) Vermicomposts and compost effect on plant growth in horticulture container media and soil. Pedobiologia (44) 579-590.
6. Banu JR, Logakanthi S, Vijaylakshmi GS (2001) Biomanagement of paper mill sludge using an indigenous (lampitomauritii) and two exotic species of earthworm (i.e., Eudrilus Eugenie and Eiseniafoetida). J Environ Biol (22) 181-185.
7. Bansal S, Kapoor KK (2000) To study vermicomposting of crop residue cattle dung using Eiseniafoetida. BioresourceTechnol (73) 95-98.
8. Benitez E, Nogales R, Elvira C, Masciandaro G, Ceccanti B (1999) Enzyme activity acts as an indicator of stabilization during vermicomposting of sweage sludge. BioresourceTechnol (67) 279-303.
9. Bhatanagar RK, Palta RK (1996) A study on vermiculture and vermicomposting. Kalyani Publishers, New Delhi.
10. Brown BA, Mitchell MJ (1981) To study the role of earthworm, Eseniafetida, in affecting the survival of Salmonella enteritidisSer.Typhimurium. Pedobiologia (22) 434-438.
11. Brown GG, Barois I, Lavelle P (2000) To study the regulation of soil organic matter and microbial activity in the drilosphere and the role of interaction with other edaphic functional domains. Eur J Soil Biol (36) 177-198.
12. Butt KR (1993) utilization of solid paper mill sludge and spent brewery yeast as a feed for earthworm. BioresourceTechnol (44) 105-107.
13. Chan LPS, Griffiths BA (1988) Vermicomposting using perpetrated pig manure .Biol Waste (24) 57-69.
14. Dominguez J, Edwards CA (2004) A review of vermicomposting organic waste. In Shakir Hanna SH, Mikhail WZA (eds) Soil Zoology for sustainable Development in the 21st century, Cairo,pp 369-395.
15. EdwardscA, Bohlen PJ (1996) A study of biology and ecology of earthworms. Chapman and Hall, London, P 426.
16. Edwards cA (1998) To study the activity of earthworm in the breakdown and management of organic wastes. In: Edwards CA (ed) Earthworm Ecology. CRc Press, Boaco Raton, PP 327-354.
17. Edwards CA Burrows I, Flether KE, Jones BA (1985) The effect of earthworms in composting farm wastes. In: Gasser JKR (ed) composting Agricultural and Other wastes. Elsevier, London, PP 229-241.
18. Elvira C, Dominguez J, Sampedro L, Mato S (1995) Vermicomposting using wastes of pulp industry. Biocycle (36) 62-63.
19. Elvira C, Sampedro L, Dominguez J, Mato S (1997) To study the vermicomposting process of wastewater sludge from paper pulp industy with nitrogen rich materials .Soil BiolBiochem (9) 759-762 .
20. Esakkimmal .B and L .Lakshmibai, (2013).Study of bacterial population in the gut region of Eudriluseugeniae.Int.J.Curr.Microbiol .App.Sci.2 (5):267-270.
21. Fracchia L, Dohrmann AB, Nartinotti MG, Tebbe cc (2006) Bacterial diversity in a finished compost and vermicompost by PcR amplification of 16srRNA gene .ApplMicrobiolBiotechnol (71) 942-952.
22. Franke-Whittle, I. H. Knapp, B.A. Fuchs, J, Kaufmann, R. and Insam, H (2009) Application of compo chip microarray to investigate the bacterial communities of different composts. Micro Ecol 57, 510-521.
23. Gajalakshmi ,Ramasamy EV, Abbasi SA (2002) Vermicomposting of paper waste with the anecic earthworm LampitomauritiiKingburg .Indian J chemtechnol (9) 306-311.
24. Gandhi M, Sangwan V, Kapoor KK, Dilbaghi N (1997) A study on composting of household waste with and without earthworm. Environ Ecol (15) 432-434.
25. Hartenstein R, Neuhauser EF, Kaelan DL (1979) A study on reproductivy capacity of earthworm *Eiseniafoetida* .Oceologia (43) 329-340.
26. Huang et al. (2013) changes of bacterial and fungal community composition during vermicomposting of vegetable wastes by Eiseniafoetida. BioresourTechnol 150, 235-241.
27. Ismail SA (1997) Study on biology of earthworm. Orient Longman Limited, Chennai.
28. Kale RD, Bano K (1988) A studies on vermiculture technique for the production of vee cOMP83E USA. Mysore J AgricSci (2) 339-344.

29. Kooch Y, Jalilvand H (2008) Earthworm as ecosystem engineers and the most important detrivors in forst soil. Pak J Boil Sci (11) 819-825.
30. Lee KE (1985) Earthworm's ecology and their relationship with soils and land use. Academic Press, Sydney.
31. Lavelle P, Martin A (1992) Large-scale and small-scale effects of endogeic earthworms on soil organic matter dynamics in soils of the humid tropics soil. BiolBiochem (12) 1491-1498.
32. Lazcano c, Gomez-Brandon M, Dominguez J (2008) A comparative study on effectiveness of composting and vermicomposting for the biological stabilization of cattle manure. Chemosphere (72) 1013-1019.
33. Lv, B. Xing, M. and Jang, J. (2015) to study the effect of bacterial profiles during vermicomposting of sewage sludge and cattle dung with high throughout put of sequencing.Appl N Microbial Biotechnol 99, 10703-10712.
34. Maboeta MS, Van Rensburg L (2003) Vermicomposting using industrially produced wood chips and sewage sludge using Eiseniafoetida. Ecotoxicol Environ Saf (56) 265-270.
35. Munnoli PM, Da Silva JAT, Saroj B (2010) A review: on the dynamics of soil earthworm and plant relationship. Dynamic soil, dynamic 1-21.
36. Nakamura Y (1996) To study the interaction between earthworms and microorganisms in biological control of plant root pathogens. Farming Jpn (30) 37-43.
37. Ndegwa PM, Thompspon SA, Das Kc (2000) Effects of stocking density and feeding rate on vermicomposting of biosolids. BiiresourTechnol (71) 5-12.
38. Parthasarathi K, Ranganathan LS (1998) PressmudzaVermicast as a hotspot for fungi and bacteria. Ecol Environ Cons (4) 81-86.
39. Pathma J, Rahul GR, Kamaraj Kennedy R, Subashri R, Sakthivel N (2011b) To study the secondary metabolities production by bacteria antagonists. Journal of Biological Control (25) 165-181.
40. Pedersen JC, Hendriksen NB (1993) Effect of passage through the intenstinal tract of detrivore earthworms i,e. lumbricus species on the no of selected gram negative bacteria and total no of bacteria. BiolFertil Soils (16) 227-232.
41. Petersen H, Luxton MA (1982) A comparative analysis of soil funnapoplution and their role in decomposition process. Oikos (39) 287-388.
42. Prakash, M., and Hemalantha, N.(2013) .Microorganisms during vermistabilisation of organic substrates increases the activity of PGPR bacteria on Black gram.
43. R. Gopinatha and M. Prakash (2014).Isolation of Plant Growth Promoting Rhizobacteria (PGPR) from vermicompost and effect on growth of green gram. Int .J. curr. Microbio. App .Sci 3(7) 1072-1081.
44. Reeh U (1992) To study the influence of population densities on growth and reproduction of the earthworm Eisenia Andrei on pig manure. Soil BiolBiochem (24) 1327-1331.
45. Senappathi K, M. C. Dash, A. K. Pana and Panda, B. K. (1980) To study the effect of earthworm in the decomposition process in soil under laboratory condition. Comp. physic. Ecol. 5:140-142 .
46. Shrama S, Pradhan K, Satya S, Vasudevan P (2005) A review on potentiality of earthworms for waste-management and in other uses. The Joumal of American Science (1) 4-16.
47. Sinha RK, Heart S, Agarwal S, Asadi R carretero E (2002) Study of vermiculture technology for environmental management and action of earthworms Eiseniafoetida, Eduriluseugeniae and Perionyx excavates on biodegration of some community wastes in India and Astrulia. The Envirnomentalist (22) 261-268.
48. Subler S, Edwards CA, Metzger PJ (1998) Comparison study of composts and vermicomposts. Biocycle (39) 63-66.
49. Suthar S, Singh S (2008) To study the vermicomposting of domestic wastes by using two epigeic species earthworm i,e. Perionyxexcavatus and Perionyxsansibaricus. Int J EvnironSci and Technol (5) 99-106.
50. Tajbakhsh J, Abdoli MA, MohammadiGoltapeh E, Alahdadi I, Malakouti MJ (2008) Study on physcio-chemical properties change in recycling spent mushroom compost through vermicomposting by epigeic earthworms Eiseniafoetida and Eisenia Andrei. AgricTechnol (4) 185-198.
51. Vivas A, Moreno B, Garcia-Rodriguez S, Benitez E (2009) Study the impact of composting and vermicomposting on bacterial community size and structure and functional diversity of olive-mill waste. BioresourTechnol (100) 1319-1326.

52. Yasir M, Aslam Z, Kim SW, Lee Sw, Jeon CO, Chung YR (2009a) Dection of bacterial community composition and chitinase gene diversity of vermicompost with antifungal activity. BioresourTechnol (100) 4396-4403.

Table 1.Effect of vermicomposting bacteria on growth rate and yielding capacity of green gram.

Type of soil	No of days	Shoot length in (cm)	Root length in (cm)	No of root hairs	No of branches	No of leaves	No of flowers	No of pods
T 1	10 days	3.5	2.5	9	0	0	0	0
T2		6.5	3.2	13	0	0	0	0
T3		6.7	3.9	15	0	0	0	0
T4		4.9	2.9	11	0	0	0	0
T1	20 days	9.8	5.7	29	0	0	0	0
T2		11.2	7.5	34	1	3	0	0
T3		12.4	8.1	35	2	6	0	0
T4		10.7	6.8	32	0	0	0	0
T1	30 days	14.9	8.2	48	0	0	0	0
T2		16.2	10.2	55	2	6	2	0
T3		16.9	10.9	69	3	9	3	0
T4		15.8	9.7	50	1	3	1	0
T1	40 days	17.9	12.7	69	2	6	1	0
T2		20.1	14.5	77	4	12	4	2
T3		20.9	14.9	78	5	15	5	3
T4		19.7	13.8	72	3	9	2	1
T1	50 days	19.9	15.9	76	5	15	5	1
T2		22.7	17.6	81	8	24	7	4
T3		25.9	18.1	85	9	27	9	5
T4		21.8	16.9	77	7	21	6	3
T1	60 days	25.6	14.8	85	7	21	6	3
T2		28.9	18.7	93	10	30	10	6
T3		30.7	19.5	97	12	36	12	7
T4		27.3	15.9	89	9	27	8	4
MEAN		17.12083	11.37083	57.45833	3.75	11.25	3.375	1.625
SD		7.7541	5.450766	28.62802	3.779234	11.3377	3.739478	2.203012

T1= Composting soil **T2**= Composting soil treated with vermicomposting bacteria broth,
T3 = Vermicomposting soil, **T4**= Composting soil treated with only nutrient broth.

Table 2. Types of colony observed in treated composting and vermicomposting soil

Type of soil	Total CFU/ml	Total no Type of bacterial colony	Type of bacterial colony
T2 Composting soil treated with bacterial spray of vermicomposting	$18x10^5$/ml	2	Small white glassy colony
			Irregular yellow mate colony

T3 Vermicomposting soil	27x1o^5/ml	4	Big Rounded White Glassy colony
			Small yellow Rounded Glassy Colony
			Rhizoid white Mate colony
			Small White Glassy colony

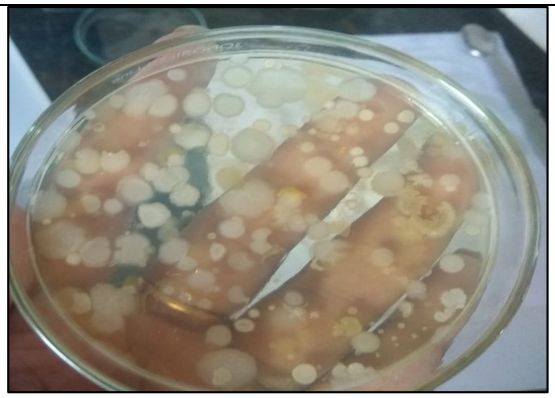


Figure. 1.Bacteria cultured from vermicomposting soil.

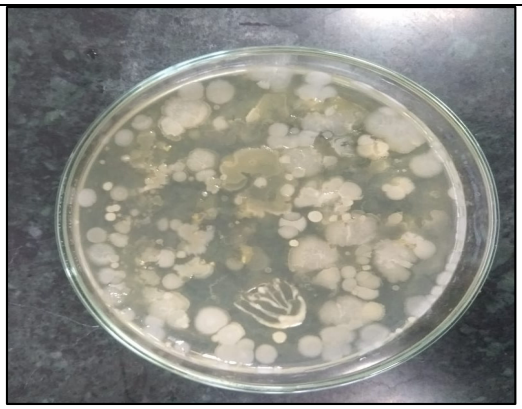


Figure. 2. Bacteria cultured from composting soil

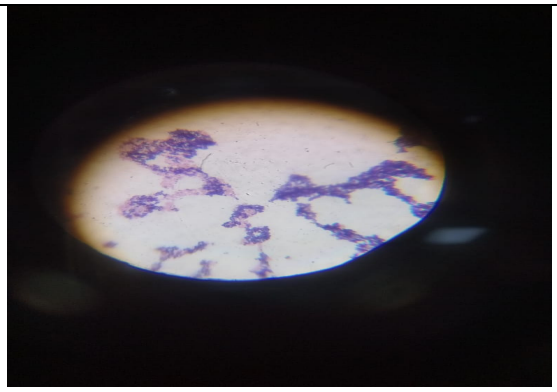


Figure. 3.Gram +ve BWG colony

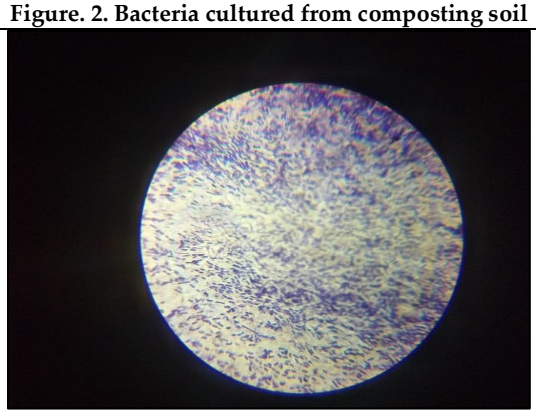


Figure. 4. Gram +ve SYG colony

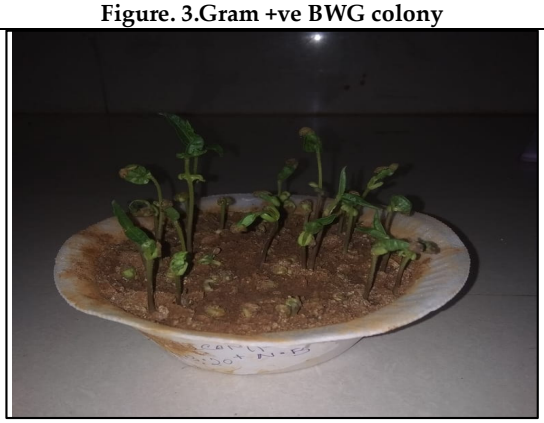
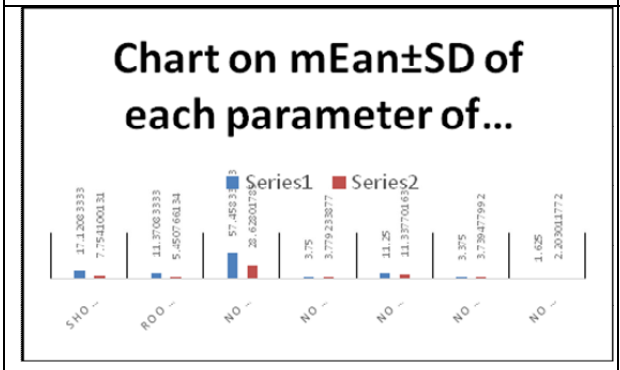


Figure. 5.Composting soil—T1

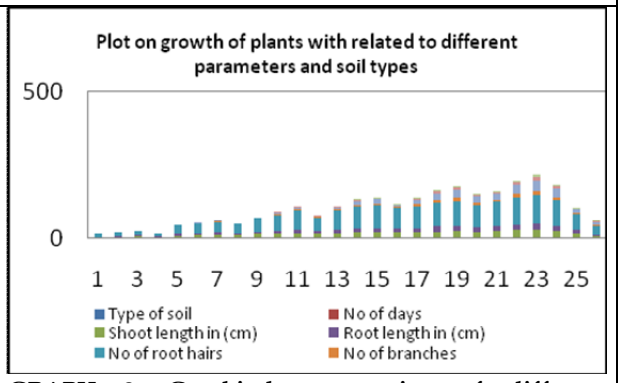
Figure. 6.Vermicomposting soil—T2

Figure. 7.Composting soil treated with nutrient broth ---T4

Figure. 8.Composting soil treated with vermin composting bacteria---T3



GRAPH 1. Graphical presentation of different growth parameters during vermicomposting and treated bacterial composting soil with mean±SD



GRAPH 2. Graphical presentation of different parameters of growth observed in all treated pots

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RESEARCH ARTICLE

Supplement of Biowaste (Egg Shell) as Nutrition in Vermiculture and Its Effect on earthworm *Eudrillus eugeniae*

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ABSTRACT

Production of different types of wastes is rapidly increased in the last few years due to the urbanization and industrialization. Different techniques has been applied to dispose wastes through different processes of recycling method where maximum wastes can be used for the agricultural purposes, Recycling of waste materials for agriculture purposes decreases the use of chemical fertilizers and increases the filled of organic fertilizers. The objective of the present study is to find the possibility of utilization of disposal eggshell from the kitchen through vermicomposting by increasing the population of vermireactor *Eudrillus eugeniae*in the process of vermiculture.It is at least a century years old but it is now used worldwide for the management of waste substances. The earthworm increases nutrient availability, better drainage, and more stable soil structure. Higher feeding, growth and biodegradation capacity in soil was found in the species *E. eugeniae*. Enhancement in natural biodegradation and decomposition of wastes was shown by the action of earthworm within 70-80days.The degradation of all the waste were taken in the study achieved with increasing in physical growth as well as population growth of the earthworm after consumption as nutrition.

Keywords: *Eudrillus eugeniae*, Egg shell (ES), Physico-chemical parameters,Vermicomposting (VC)

INTRODUCTION

Organic waste contains materials that are biodegradable and originated from the living organism can be broken into carbon dioxide, methane, or simple organic molecules. Organic materials found in municipal solid waste include food, paper, wood, sewage sludge, and yard waste. Like most waste materials eggshells are one of these obtained

from hatcheries, domestic use, canteens, hostels, hotels, fast food centers, factories and industries (Phil and Zhihong, 2009; Amu et al., 2005) and can be readily collected in plenty. Eggshell waste disposal contributes to environmental pollution. Challenges associated with the disposal of eggshells include cost, availability of disposal sites, odor, flies and abrasiveness (Phil and Zhihong, 2009). However, they can be processed into saleable products like fertilizer, used in artwork, human and animal nutrition, and building materials and to produce collagen from the membranes (Phil and Zhihong, 2009; Amu et al., 2005).

The egg shell is composed of approximately 98.2, 0.9, 0.9% amount of calcium carbonate, magnesium and phosphorus (phosphate) respectively (Romanoff et al., 1949). Eggshells contain calcium and trace amounts of the micro elements i.e. magnesium, boron, copper, iron, manganese, sulphur bi silicon and zinc (Bee, 2011). Eggshell calcium is probably the best natural source of calcium and it is about 90% absorbable (Bee,2011). It is a much better source of calcium than limestone or coral sources. Shell membranes comprises of approximately 10% collagen (Froning 1998) that is extracted and has diverse uses in medicine, biochemical, pharmaceutical, food, and cosmetics industries. These uses minimize their effect on environmental pollution. The eggshell comprises of calcified shell and shell membranes including inner and outer members developed a patent for separating eggshell membranes(Mac Neil,1997). Besides throwing the eggshell improves the soil in the garden, as it is a good source of calcium for plants and can help make a great fertilizer improves soil quality.

Verrmiculture (derived from the word Latin vermis meaning worm) involves the mass production ofthe earthworms for waste degradation and compositing with vermicast production. Vermi culture appears to be an innovative sustainable technology for waste materials which holds a promising future in the field of organic waste management the technology of vermiculture can effectively manage the waste. Earthworms are terrestrial invertebrates belonging to the Order Oligochaeta, Class Chaetopoda, Phylum Annelida, which have originated about 600 million years ago, during the pre-Cambrian era (Piearce et al., 1990). There are about 3000 varieties of earthworms. They have been formally classified into main 3 types based on their lifestyles and burrowing habits. Earthworms are long, narrow, cylindrical, bilaterally symmetrical, segmented animals without bones. The body is dark brown, glistening and covered with delicate cuticle. Earthworms are burrowing animals and form tunnels by literally eating their way through the soil. Earthworms are generally absent or rare in soil with a very coarse texture in soil and high clay content or soil with pH < 4 (Gunathilagraj, 1996).

MATERIALS AND METHODS

Collection of Materials

The present experimental study on vermiculture was carried out approximately about 70-80days for the duration of January to March (2020) on the campus of CUTM, located at Jatni Bhubaneswar, Odisha, India.Collection of materials soils, cow dung, eggshell were carried out of CUTM campus. The soil was collected from the garden area of the CUTM campus. Cow dung was collected in large-sized plastic containers from cattle shed of the CUTM campus. Eggshell was collected from the canteen area of the CUTM campus. The species *Eudrilus eugeniae* was used for vermiculture. Earthworms were collected from the vermiculture center of CUTM.

Preparation for experiment

The collected materialwere allowed for drying on sunlight, crushing and then sieving. The dried and sieved materials were weighed into 6 different proportions labelled as control (1:1), L1 (4:1), L2 (3:2), L3 (2:3), L4 (1:4), ESw (100%) as experimental by taking 6 rectangular plastic pots. All the materials were mixed properly and allowed to add water by sprinkling upto reach moisture uniformly throughout the containers. The mixture is allowed for precomposting for a week before set up to vermicomposting

Introduction of Earthworm

The process of vermicomposting was started in the present study by introducingearthworms into the pot. Each pot was supplied with 3 earthworms *Eudrilus eugeniae* of various length.

Culture of Earthworm

The earthworms in the potswere maintained by regular addition of water and cow dung slurry within time interval for their moisture content and room temperature as same as atmospheric temperature. In initial stage the earthworm *Eudrilus eugeniae*was not survived in L4 and experimental then adopted to produce population.

Process of Vermicomposting

In the favorable environment the earthworms were started to reproduce juveniles after consuming the waste to grow and survive. Due to the physiological action of earthworm *Eudrilus eugeniae* thatthe waste converted to vermicompost after releasing of vermicasts. In regular interval of time sprinkling of water was carried out every day in the preliminary stage of vermicomposting and in the due period of processing it was repeatedly done within 4-5 days of gap to maintain moisture regularly. Regular monitoring of vermicomposting process was observed and recorded till the process was conducted for 70-80 days.

Harvesting of Earthworm

In order to facilitate the separation of worms from vermicomposting, the moisture content in the compost is brought down by stopping the addition of water for 4-5 days before maturation that ensures drying of compost a migration of worms into vermiculture pot. The remaining worms can be removed by hand. The mature compost is removed out from the pot, dried and packed for use in plant growth.

RESULTS AND DISCUSSION

From the present study like other waste, eggshell was used as an organic substrate with soil and cow dung in different proportions and especially it was treated as nutrition. During vermiculture the eggshell along with soil and cow dung was consumed and passing through gizzard later released vermicasts. The survival rate was increased depending upon the growth and capacity of reproduction due tophysiochemical variables temperature, electro-conductivity, pH and water holding capacity (moisture content) were also observed as the following table and graphs. Each proportion varies with their physico–chemical variables studied and observed with respect to electro conductivity, pH, temperature and moisture content. The pH value of each proportion mixed with eggshell powder in this experiment was ranged from 6.5 to 7.8 where the eggshell mixture reduced the acidity of soil may due to presence of rich calcium .It was shown in Table-1 and Fig.1-4 that the slightly acidic soil when mixed with eggshell powder converted towards alkaline may be addition with cow dung during the process of vermicomposting with combining action of microbes and earthworms changed the pH towards alkaline within 7.5 which is suitable for survival of earthworm and plant growth((Nisha Jain,2016))The electro-conductivity was increased from the initial value during vermicomposting might have added salinity to each proportion due to composting of calcium carbonate of egg shell. The moisture content was slowly increased due to the physical action of earthworm in vermibed and the temperature was maintained below 35^0C that indicated the survival and enhanced the earthworm population (Table-2& 3) which yielded with faster vermicompost. The suitable vermiculture rate was observed in L1 and L2 with response to control and also shown in 100% eggshell proportion. It was observed that in almost all proportion the population was achieved represented in (Fig 5& 6).

CONCLUSION

From the present study it was carried out within 70 to80 days that the earthworm was grown in their physical appearance as well as their population that increased. It was observed that the population growth of earthworm was found in all proportion of eggshell but more in lower proportion as well in 100% also comparison to others. The organic solid waste when feeding by earthworm including microorganisms converted into brownish powdery called vermicompost. It was observed that for each physico-chemical variable, the collected data after laboratory work converted to fine vermicasts having an increased level than initial reading which indicated the enhancement in plant growth.

REFERENCES

1. Agarwal, S., Sinha, R.K. and Sharma, J. (2010) 'Vermiculture for sustainable horticulture agronomic impact studies of earthworms, cow dung compost, and vermicompost vis-à-vis chemical fertilizers on growth and yield of lady's finger (Abelmoschus esculentus)', Int. J. Global Environmental Issues, Vol. 10, Nos. 3/4, pp.366–377.
2. Ansari, A. A., & Ismail, S. A. (2012). Earthworms and vermiculture biotechnology. *Management of Organic Waste, Eds) by Sunil Kumar and Ajay Bharti*, 87-96
3. Amu, O. O., Fajobi, A. B., & Oke, B. O. (2005). Effect of eggshell powder on the stabilizing potential of lime on expansive clay soil. *Journal of Applied Sciences*, *5*(8), 1474-1478.
4. Burley, R. W., & Vadehra, D. V. (1989). The eggshell and shell membranes: properties and synthesis. *The Avian Egg, Chemistry and Biology. John Wiley, New York*, 25-64.
5. Froning, G. W. (1998). Recent advances in egg product research and development.
6. Gunathilagraj, K. and Ramesh, P.T. (1996) Degradation of coir wastes and tapioca peels by earthworms; Training Program in Vermiculture; Indian Council of Agricultural Research (ICAR), New Delhi.
7. Gunathilagraj, K and T, Ravignanam (1996) Vermicomposting of sericultural wastes; Madras Agricultural Journal; Coimbatore, India; pp. 455-457.
8. Hemalatha, B. (2013). Vermiculture for organic waste. *International Journal of Advanced Engineering Technology*, *4*(1), 46-47.
9. Kale, R. (1991) Vermiculture: Scope for New Biotechnology Zoological Survey of India, Pub., Calcutta.
10. King'Ori, A. M. (2011). A review of the uses of poultry eggshells and shell membranes. *International Journal of Poultry Science*, *10*(11), 908-912.
11. MacNeil, J. (1997, September). Separation and utilization of waste eggshells. In *Proceedings of the International Egg Commission Annual Production and Marketing Conference, Toronto, ON, Canada* (Vol. 30).
12. Nakano, T., Ikawa, N. I., & Ozimek, L. (2003). Chemical composition of chicken eggshell and shell membranes. *Poultry Science*, *82*(3), 510-514.
13. Piearce, T. G., Oates, K., & Carruthers, W. J. (1990). A fossil earthworm embryo (Oligochaeta) from beneath a Late Bronze Age midden at Potterne, Wiltshire, UK. *Journal of Zoology*, *220*(4), 537-542.
14. Phil, G., & Zhihong, M. (2009). High-value products from hatchery waste. *RIRDC publication*, (09/061).
15. Romanoff, A. L., & Romanoff, A. J. (1949). The avian egg. *The avian egg.*
16. Shuster, W. D., Subler, S., & McCoy, E. L. (2000). Foraging by deep-burrowing earthworms degrades surface soil structure of a fluventic Hapludoll in Ohio. *Soil and Tillage Research*, *54*(3-4), 179-189.
17. Sinha, R. K., Herat, S., Agarwal, S., Asadi, R., & Carretero, E. (2002). Vermiculture and waste management: the study of the action of earthworms Elsinia foetida, Eudrilus eugeniae and Perionyx excavatus on biodegradation of some community wastes in India and Australia. *Environmentalist*, *22*(3), 261-268.
18. Soni, R., & Sharma, A. (2016). Vermiculture technology: a novel approach in organic farming. *Indian Horticulture Journal*, *6*(1), 150-154.

TABULATION-1

Sl No.	Observation	Electro-conductivity			pH			Moisture content			Temperature ^{0}C	
	Experimental set ups	Initial	Final	Difference	Initial	Final	Diff.	Before vermi compost	After vermicompost	Diff.	Initial	Final
1	Control	0.713	0.936	0.223	6.9	7.2	0.3	0.391	0.487	0.96	32.5	31
2	L1	0.250	0.549	0.299	6.81	7.23	0.42	0.163	0.288	0.125	30.8	28.7
3	L2	0.364	0.712	0.348	6.93	7.25	0.32	0.173	0.295	0.122	30.6	28.9
4	L3	0.441	0.965	0.524	6.87	7.29	0.42	0.292	0.329	0.137	30.7	29
5	L4	0.746	0.984	0.238	7.48	7.26	0.22	0.446	0.495	0.049	31.5	29.9
6	Expt.	0.342	0.529	0.187	7.68	7.44	0.24	0.453	0.495	0.042	32.1	30.8

TABULATION-2

Sl. No.	Proportional Set up	Initial No. of earthworm	Survival of earthworm In 15 days	Survival of earthworm in 2nd 15 days	Survival of earthworm in 3rd 15 days	Survival of earthworm in 4th 15 days
1.	Control (1:1)	3	7	13	17	26
2.	L1 (4:1)	3	5	7	11	19
3.	L2(3:2)	3	4	5	10	13
4.	L3 (2:3)	3	4	5	6	11
5.	L4 (1:4)	3	3	4	6	9
6.	Expt.(100%)	3	3	7	12	16

TABULATION-3

Experimental setup	No. of Earthworm introduced	Length(in cm)		Diameter(in cm)		Perimeter(in cm)	
		Mean	SD	Mean	SD	Mean	SD
C	3	3.22	0.21	0.2	0.14	0.6	0.35
L_1	3	2.35	0.45	0.2	0.082	0.575	0.23
L_2	3	2.22	0.917	0.275	0.216	1.6	1.34
L_3	3	2.46	0.485	0.2	0.116	0.65	0.19
L_4	3	2.93	0.877	0.225	0.093	0.75	0.32
E	3	5.61	1.46	0.575	0.05	1.97	0.38

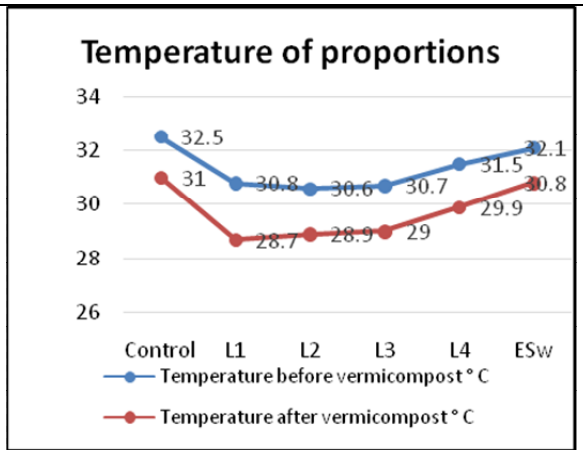

Fig.1. Graphical presentation of Temp. during vermicomposting

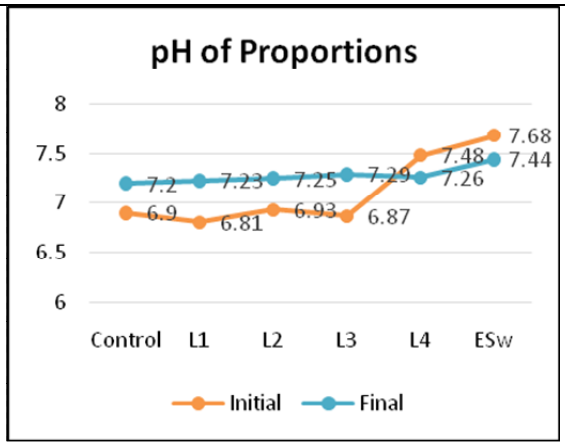

Fig.2. Graphical presentation of pH during vermicomposting

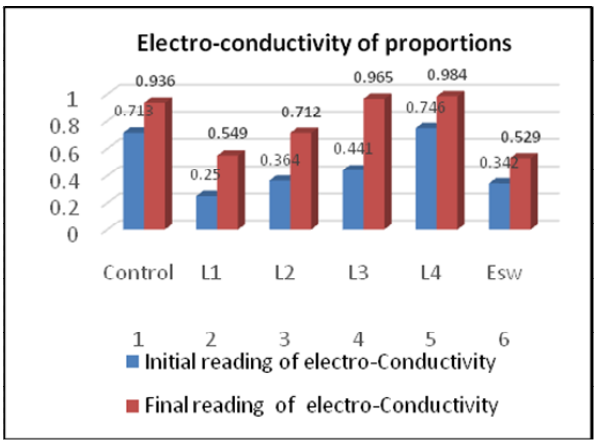

Fig.3. Graphical presentation of electro-conductivity during vermicomposting

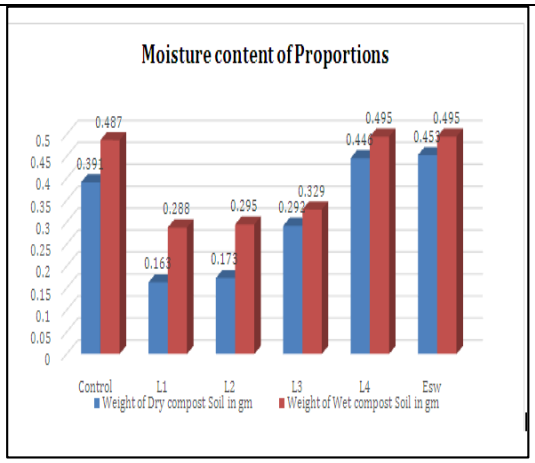

Fig.4. Graphical presentation of moisture -content during vermicomposting

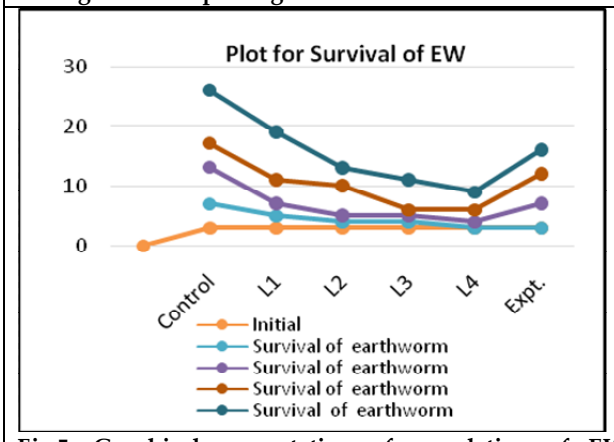

Fig.5. Graphical presentation of population of EW during vermiculture

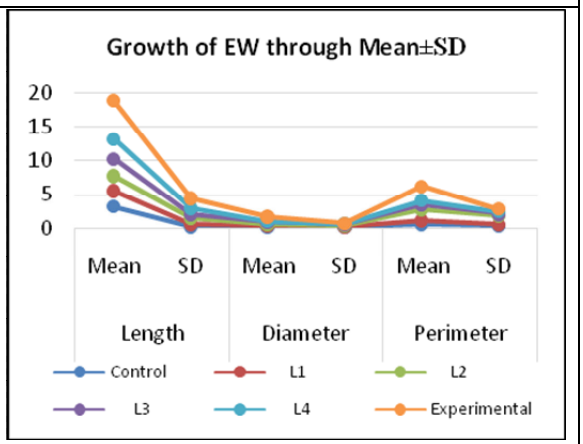

Fig.6. Graphical presentation of growth during vermiculturegrowth

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RESEARCH ARTICLE

Potential Use of Pulse Waste of Pigeon Pea- (*Cajanus cajan)* as a Nutrient in Vermiculture and it's Effect on Growth of *Eisenia foetida*

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ABSTRACT

Conversion of organic wastes into enriched nutrient for enhance soil fertility and sustainable plant growth is the challenge of present days for contribution towards recycling and agricultural production. According to food and agriculture organization (FAO) of the UN, about one third of the food produced for the human consumption ,which amount to 1.3 billion tones roughly 30% of global food production , is lost or wasted annually .Wedding , events , restaurants , hostels ,temples and houses are a major sources for food wastage of cooked food. Enormous production of organic wastes coupled with poor management system, results in a significant environmental degradation. The amount of pulses waste in India is above 450MT/day.Vast amount of dal are being wastes everyday from hostels, hotels, houses, weddings, various educational institutes and other events. For reducing the wastage of pulses and diminish the environmental degradation, Organic manure provides a solution to the alarming environmental damage is vermitechnology. The vermicomposting is a process of treating organic waste in to worth organic manure as needed for the crops by the action of earthworms. The production of earthworms in vermibed faster the rate of vermicomposting along with the microbial activities. In present study different proportion of mixture of soil, cattle dung and waste pulses (cooked) were taken and conducted vermiculturing process using exotic species *Eisenia foetida* to monitor the population growth and involvement of the worms in production of vermicompost. The study was estimated by measuring various physico-chemical parameters of initial and final process of vermiculture in the supplied environment.

Keywords: Organic waste, Pulse wastes, Vermiculture, *Eisenia foetida*

INTRODUCTION

Any substances which discarded after primary use, or worthless, defective or of no use and produced huge amount in form of organic or inorganic materials are considered as wastes. The production sources of wastes are due to urbanization and industrialization towards fulfillment of the demand of humankind in the present day. India generates as much as 25 million tons of municipal solid wastes, 320 million tons of agricultural waste 210 million tons of cattle manure and 3.3.million tons of poultry manure and food wastage is a global problem. Approximately one third of the food produced for the human consumption, which amounts to 1.3 billion tons, get wasted annually is reported according to the Food and Agriculture Organization (FAO) of UN. It is estimated by the UN that nearly 40% of food wasted that produced in India. Celebration events, restaurants, hostels, NGOs, holy places and houses are the major sources of food wastage of cooked food. These organic wastes if not treated in timely and effective manners these organic wastes not only takes up much available land, cause environmental pollution and harm human health. Such varied types of solid waste can be converted into useful and worth product such organic manure, needs for the plants to grow and develop. As a vast amount of cooked pulses (dal) being waste daily from different sources by means of leftover, unused dal, ruminative dal etc .

It can be converted these wastes to wealth by subjecting them into any kind of bio conversion option. *Eisenia foetida* are known as the best species used for vermicomposting and vermiculture. *Eisenia foetida* known under various common name such as red worm, trout worm, brandling warm, tiger worm etc. The behavior of it studied from literatures state that these adapted to decaying organic material and thrive in rotting vegetation, compost and manure. They are epigean that rarely found in soil that move in and out to gripe nearby surface as the worms stretch and contract. They are also known as biological indicator or silent machines of soil fertility that have been performing a marvelous function of ploughing and fertilizing soils .When earthworms are available in soils they alter soil porosity, increase in soil air volume from 85 % to 30%.and promote plant growth.

Vermicomposting is one of the biological treatments of solid waste into useful manure which is an aerobics organic wastes into humus. Vermicomposting cleans the environment and provide ruminative organic manure and it is 100% organic, non-toxic and odour free. The worms feeds on organic materials, breakdown into simpler form in the body and excrete it as casting or vermicompost. This castings are look like tiny pellets coated with gel which ultimately helps in improving the quality of soil drainage and aeration. Vermiculture is the scientific method of breeding and raising the population of earthworms in controlled medium which feeds on waste materials and soil there by releasing digested food material back into the soil, thus producing compost rich nutrient . Vermiculture a promising source of biofertilizer (Bhawalker ,1989) and it is clearing up environment with cost effective management technology contribution in the field of vermicompost (Sultan Ismail,1993 and Guna Thilagaraj,1994). The present experimental work is to enhance the population rate of *Eisenia foetida* in vermiculture process so that the production of vermicompost by recycling of pulse waste can be accelerated and the observation for the organic fertilizer which is obtained from the pulse waste estimated through different physico-chemical parameters.

MATERIALS AND METHODS

The present experimental study on vermiculture was carried out approximately about 60-70 days from January to March in the campus of CUTM located at Jatni, Bhubaneswar, Odisha, India.

Collection of Samples

Collection of samples such as soils, cow dung was carried out from farming area of CUTM, India. The cooked pulse waste was used as nutrients for vermiculture bed collected from the canteen of of girls' hostel, CUTM campus. Urine free cow dung was collected in a large sized rectangular plastic container from the cattle shed of the campus .More than required amount of soil was collected from the garden area of the campus .The exotic healthy species *Eisenia foetida* was used for the purpose of vermiculture were picked up from the vermiculture unit of the campus.

Rectangular plastic pot with 27 cm in length, 20cm in breadth and 18cm in height from the bottom to the top were collected from the market for vermiculture.

Preparation for Vermiculture Mixture

The collected cow dung and soil were exposed in bright sun light for air drying and observation for drying was monitored everyday in a regular basis. The large pieces of cow dung and soil were chopped into small pieces and was allowed for further dry. The required cow dung and soil were completely dried and were again honked and chunked into smaller particles .The dried materials were sieved initially through a sieve having diameter 2.36 and after that the materials were brought into weighing site for the accurate measurement of the materials into different proportion of 20%,40%,60%,80% and 100% of pulse wastes

Experimental Setup

The experimental was designed with the following proportion by taking 6 rectangular pots labelled as

Control =	Control (soil + cow dung)	(1:1)
Proportion-1 =	Soil + cow dung + w.pl	(4:1)
Proportion-2 =	Soil + cow dung + w.pl	(3:2)
Proportion-3 =	Soil + cow dung + w.pl	(2:3)
Proportion-4 =	Soil + cow dung + w.pl	(1:4)
Experimental=	(100%-w.pulses)	

The various proportion of mixture samples were taken in different labelled pots and kept in shaded area. Sprinkling of water was done daily upto 10 – 15 days to maintain moisture content.

Introduction of Earthworm

After slight decomposition of the composting materials i.e. after 25days about 3-4 earthworms of exotic species *E. foetida*, having length between 7-12cm are introduced into composting.

Culture of Earthworm

The earthworm were allotted into all different pots and cow dung slurry were administrated to the pots for maintain their nutrition for earthworm. Water was allowed to sprinkle in regular interval to all proportion for maintaining moisture content and the room temperature is also maintaining as same as atmospheric temperature.

Harvesting of Earthworm

In order to facilitate the separation of worms from vermicomposting, the moisture content in the compost was brought down before 4-5 days of harvesting that ensure drying of compost and migration of worms into vermiculturing pot. The remaining worm can be removed by hand. The mature compost is removed out from the pot, dried and packed.

RESULT AND DISCUSSION

In the present study various proportions of waste pulses was experimented by using vermicomposting for production of enriched organic manure. The physico-chemical parameters like pH, moisture content and electroconductivity were easily controlled and indicated the progress of vermicomposting. Graphical analysis of pH, electro-conductivity and moisture content were studied in Table 1. And figs. (1.,2,3&4) . Each proportion from the present work was found varies with their physio–chemical variables, which studied and observed with respect to elecrto-conductivity,pH and moisture content. The output with better result was observed in both Proportion-1 and Proportion-2 as compared to other pots in respect to all physico-chemical parameters. Rapid consumption of organic pulse wastes by earthworm crushed into finer particle through gizzard the muscular grinding organ and released dark black granular vermicast (Lakshmi Prabha et al 2014). The earthworms were obtained their nutrition from microorganism during vermicomposting that grow upon the wastes. During pre-composting the microbes were

produced and undergoes a process of fermentation which converted the mixtures into acidic medium then later reached to slightly acidic (Jadhav et al, 2013). The pH was maintained within 6.5 to 7.6 i.e. in vermicomposting pots from control to experriment in present experiment.The pH in all pots were slightly acidic except Proportion-3 shown alkalinity while the experimental was acidic (Table-1 & Fig.-2). It might have caused by the microbial nitrification process of nitrifying bacteria present in wastes to release volatilization of ammonical nitrogen and H+.(Eklind and Kirchmann ,2000, Singh,et al 2005).Earthworm are aerators that it emits sufficient oxygen to oxidize foul smell producing, compounds like H_2S, mercaptans, skatol, etc. to make odourless vermicompost during the process of compost formation because of the oxygen rich hemoglobin circulation through the skin of the earthworms (Nagavallemma et al , 2000) The moisture content was maintainted by sprinkling water into all pots at 65%-75% ,whereas it was more in control (Table1. & Fig.-3). The temperature was maintained below 35^0C to avoid overheating of the wastes because earthworms to this range of temperatures even for short periods cannot survive (Taiwo and Oso, 2004). The temperature in Proportion-4 and experimental of present study was shown nearer to 35^0C causes death of earthworm(Table1. & Fig.4).From preliminary stage of vermicomposting to till completion the earthworms *E. foetida* survived in almost all pots except Proportion-4 where it was rare and nil at experimental (Table2. & Fig.-5).Soil acidification (Ma et al., 1990), decrease in soil aggregate stability (Estevez et al., 1996) decrease in soil respiration (Sharma 2003), pollution of underground water and decrease in earthworm populations (Edwards and Bohlen 1996). The EC was increased in initial stage due to release of different mineral salts available in mixture for the process of precomposting. The available salts were later converted into insoluble salts which may be the reason for the reduction of EC as the vermicomposting process further progressed (Nisha Jain,2016). From this present study it was observed that the growth of earthworm was suitable with respect to all physico-chemical paramters available such as Proportion-1, Proportion-2 in maximum rate, Proportion-3 was showing with moderate value and Proportion-4,Experimntal acheived with minimum range in respect to standard proportion taken as control. The survival and growth of earthworm *E. foetida* was led to produce juveniles subjected to population growth which indicated the faster production of vermicompost in Proportion-1and Proportion-2 while less or no vermicompost was produced in other proportions of pulse waste.

CONCLUSION

The present investigation was carried out upto 60-70 days of vermiculture by using *E. foetida* taking various proportions of waste pulses. The maximum growth and population was observed in Proportion1 and Proportion2 where as a possible minimum growth was yielded in Proportion3 at the end of completion of vermicomposting process. Normal population growth was found in control but zero population was observed in Proportion-4 and Experimental due to the above reason mentioned in discussion that high and low pH converted the environment of mixture into acidic or more alkalinity which were not the survival indicator of earthworm. This present study and observation was revealed that the raw pulse waste directly insufficient to produce vermicompost as the survival rate of earthworm is low or zero indicated that in the minimum or rare proportion the population is possible.

REFERENCES

1. Addabdo , T.D.1995 The nematicideal effect of organic amendment: a review of literature 1982-1994 Nemendment : a review of literature 1982-1994 Nematologia Mediterranea 23:299-305
2. Albanel , E.Plaixat , J and Cebrero ,T. 1988, Chemical changes during vermicomposting (Eisenia foetida) of sheep manure mixed with cotton industrial wastes, Biology and Fertility of Soils . PP 266-269
3. Angelo AJ,Mann GE.Peanut culture uses. Am. Peanut Res. Ed. Soc. Stone Printing Co.,Raonote USA,1973,561.
4. Atlavtive O and Daciulyte , j.1969 the effect of earthworms on the accumulation of vitamin B12 in soil. Pedobiologia 9:165-170
5. Bapat , P.N.Sinha , S.B and Shinde D.P.1986 Effects of S and P on yield and nutrient content of black gram J. India Soc soil Sci . 34:82-85

6. Basker , A and Macgregor , a.N 1993 Exchanneable potassium and other cations in non- ingested soil and casts of 2 species of pasture earthworms ,soil . Biol.Biochem 25:1673-1677
7. Bhagat , D.V , Yadav H.S and Dixit , J.P.1995 Effect of nutrients and growth regulators on yield and quality attribute to black gram . J.soil and Crops 5(1) :18-21.
8. Buckerfield J.C. and Webster, K.A1998 Worm-worked waste boosts grape yields : prospects for vermicompost use in vineyareds. Australian and New Zealand Wine Industry Journal 13:73-76
9. Darwin , C.1981. The formation of vegetable mould through the action of worms , with observation of their habits , Murray : London .P.326.
10. Edward , C.A Burrows , I fletcher , K.E and Jones, B.A 1985 The Use of earthworms for composting farm wastes. In Gasser J.KR(ed) composting Agricultural and other wastes Elseiver London and New York ;229-241 .
11. Edwards C.A. and Burrows, 1(1988,The potential of earthworm composts as plant growth media. In :Edwards, C.A and Neushauer, E.(eds)Earthworms in waste and Environmental management SPB Academic Press The Hauge ,The Netherlands, PP 21-32 .
12. Edwards, CA and Neuhauser, E.F 1988. Earthworms in waste and Environmental management 392 PP. SPB Academic publishings, The Hauge.
13. Edwards , C.A and Bates: J.E. 1992.The use of earthworms in environmental management Soil Biol Biochem 14(12); 1683-1689.
14. Edwards C,A and Bohlen, P.J. 1996. "Biology end Ecology of Earthworms". Third Edition 426 PP. Chapman and Hall London .
15. ELLIO. P.W.Knight. D and Anderson, J.M.1990.Denitrifiction of earthworm casts and soil from pastures under different fertilizer and draingeregimes. Soil Biol. Biochem.22(5):601-605.
16. Grappelli. A Tomati, V and Galli, E. 1985. Earthworm casting in plant propagation .Horti Sci. 20:874-876.
17. Guna thilagaraj 1994. Vermicompost for Substainable agriculture, The Hindu April-6.
18. Hopkins , W.G (E.d.),1995 .Introduction to plant wiley, New York, PP.49.
19. Jadhav, A.D. 1996 Effect of Farmyard manure and vermicompost on the yield of rice)Oryza sativa) and physicochemical propertites of Laterite soils of Kokand ,M.Sc Thesis Submitted to the KKU.Depoli.
20. Kale, R.D and Bano. K. 1986 Field trials with vermicompost (Vee ComP.E 83 VAS) an Organic fertilizer. In: Proc.Nat sem .Orga. Waste utilization vermicomposting paper II verms and vermicomposting Dash, M.C.Senapati, B.K and Mishra P.C.(eds)151-156.
21. Kale,R.D. 1998b. Earthworm Cinderalla of organic farming , Primson Books Pvt.Ltd.,Bangalore88.
22. Krishnamoorthy, R.V and Vajrabhiah, S.N 1986 Biological activity of earthworm casts.Proceedings of the Indian Academy of Science (Animal Science)95:341-351.
23. Malik JK,Singh R,Thenua OVS,Jat HS.Effect of vermicompost and biofertilizer on productivity,NUTRIENT UPTAKE AND Economic of pigeon pea Cajanus cajanmungbean 9Phaseolus radiatus0 intercropping system.Legume research.2013;36:41-48.
24. Mc.Coll, H.P. Hark, P.B.S and Cook ,F.J 1982.Influence of earth worm on some chemical propertites and the growth of eye grass on a top soil stripping .New Zwaland . J of Agri. Res. 25:239-343.
25. Neilson, R. 1965 Presence of plant growth substances in earthworms demonstrated by paper chromatography and the went Pea Test .Nature 208(5015):1113-1114.
26. Nijhawan, S.D and Kanwar , J.S 1952. Physicochemical propertites of earthworm castings and their effects on the productivity of soil .Indian J.Agri.Sci.22:257-373.
27. Orazco, F.H. Cegarra, J.Trujillo,L.M and Roig, A.1996 Vermicomposting of coffee pulp using the earhworm Eisenia foetida : effect on C and N contents and the availability of nutrients. Biology and fertility of soil 22: 162-166.
28. Parvatham ,P .1990 studies on phyto hormonal effect on Azospirillum brasilense on Brailense on Bhendhi (Abelmoschus esculenius L.Moench). M.Sc Thesis .Tamil Nadu Agricultural University coimbatore42-48.
29. Sharma, N.1986. recycling of organic wastes through earthworms for crop growth. Ph.D Thesis submitted to Indian Institute of Technology. New Delhi.

30. Shi-Wei. Z and Fu –Zhen, H .1991. the nitrogen uptake efficiency from 15N labeled chemical fertilizer in the presence of earthworm manure(cast0 In: Veeresh, G.K Rajagopal, D.Viraktmat C.A(Eds) Advances in management and conservation of Still fauna oxford and IBH publishing Co.,New Delhi, Bombay P.539-542.
31. Sultan Ismail, A1993. Composing through earthworms.Shri A.M.M Murugappa Chettiar Research Centre. Tharamani Madras MCRC Publication.
32. Vinceslas –Akpa M and Lquet , M. 1997. Organic matter transformation in lignocellulosic waste products composted or vermicomposed (Eisenia foetida anderi). Chemical analysis and CPMAS NMR spectroscopy.Soil Biol and Bichem 29:751-758.
33. V.K.Garg,R.Gupta,Effect of temperature variations on vermicomposting of household solid waste and fecundity of Eisenia foetida, Bioremediation Journal 15 (2011) 165-172.

TABULATION. 1 Measurement of Physico-chemical parameters of various observations

Sl. No	Observation	Electrocon-ductivity in S/m			pH			Moisture content			Temperature in ^{0}C	
		Initial	Final	Differe-nce	Initial	Final	Differ-ence	Before	After	Differe-ence	Initial	Final
1	Control	0.650	0.622	0.028	7.2	6.9	0.9	0.464	0.56	0.096	32.5	28.3
2	Proportion-1	0.795	0.721	0.074	6.7	6.9	0.2	0.28	0.317	0.037	30.8	28.2
3	Proportionp2	0.825	0.801	0.024	6.75	6.83	0.08	0.352	0.421	0.069	31.6	28.7
4	Proportion-3	1.454	1.42	0.034	7.7	7.4	0.23	0.479	0.520	0.044	30.7	29
5	Proportion-4	1.964	1.960	0.004	7.3	6.5	0.8	0.372	0.360	0.012	31.5	33.9
6	Expt.	2.401	2.208	0.193	6.5	6.3	0	0.423	0.419	0.004	32.1	34.8

TABULATION.2 Survival number of earthworms in each proportion during vermicomposting

Sl.No.	Propertional setup	Initial number of Earthworm	Survival of earthworm in 15days	Survival in 30days/after 1 month	Survival in 45days	Survival in 60days
1.	Control	4	5	7	13	21
2.	Proportion-1	4	4	5	9	14
3.	Proportion-2	4	4	6	9	11
4.	Proportion-3	4	4	5	3	0
5.	Proportion-4	4	2	1	0	0
6.	Experimental	4	0	0	0	0

TABULATION. 3 Growth of earthworms before and after vermicomposting in various proportion

	INTIAL		FINAL	
Experimental set ups	**Length (cm)**	**Perimeter (cm)**	**Length (cm)**	**Perimeter (cm)**
Control	7.7	0.9	8.4	1.1
	7.9	0.7	8.3	0.9
	9	1.2	9.5	1.3
	10.2	0.8	10.6	1.1
Proportion-1	7.4	0.9	7.6	1.0
	7.6	1.1	7.9	1.2
	8.2	0.7	8.4	0.9
	10.5	1.3	10.6	1.4
Proportion-2	10.2	0.8	10.3	1.0
	7.7	1.2	7.9	1.3
	8.9	0.7	9.0	0.9
	7.4	1.0	7.6	1.2
Proportion-3	8.6	0.9	8.7	1.0
	9.2	1.3	9.6	1.4
	10.1	0.8	10.3	1.2
	10.4	1.4	10.6	1.5
Propotion-4	8.4	1.3	8.5	1.3
	11.1	0.8	11.1	0.8
	10.5	0.9	10.8	0.9
	9.7	1.0	9.7	1.0
Experimental	8	0.3	1	11.9
	8	0.4	1.5	12.8
	7	0.3	1.2	14 .2
	7.5	0.1	0. 5	13.7

TABULATION. 4 Growth of earthworms presented through Mean±SD before and after vermicomposting

Experimental setup	**Length**		**Diameter**		**Perimeter**	
	Mean	**SD**	**Mean**	**SD**	**Mean**	**SD**
Control	3.22	0.21	0.2	0.14	0.6	0.35
Proportion-1	2.35	0.45	0.2	0.082	0.575	0.22
Proportion-2	2.22	0.917878	0.275	0.216	1.6	1.33
Proportion-3	2.46	0.485627	0.2	0.116	0.65	0.19
Proportion-4	2.93	0.877021	0.225	0.093	0.75	0.311
Experimental	5.61	1.463728	0.58	0.05	1.97	0.377

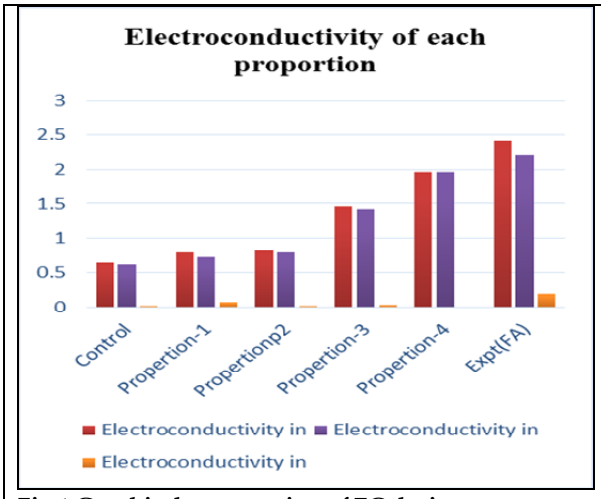

Fig.1 Graphical presentation of EC during vermicomposting

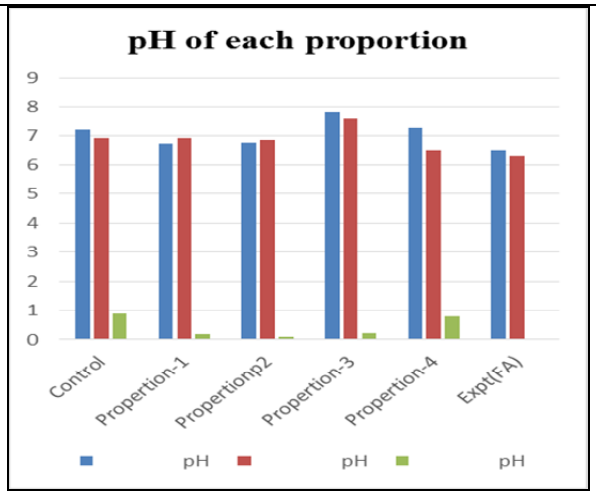

Fig.2 Graphical presentation of pH during vermicomposting

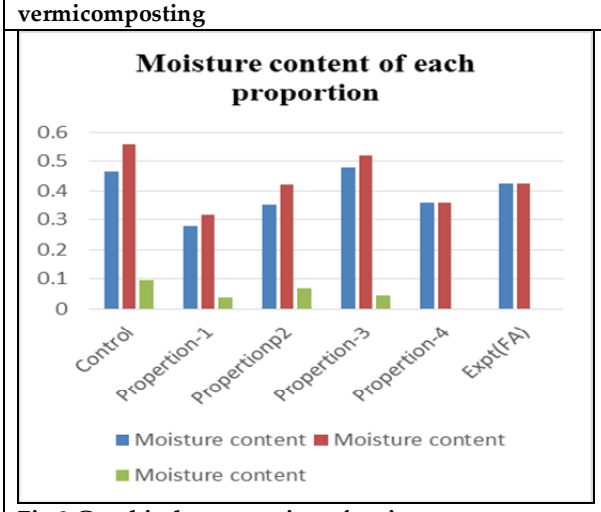

Fig.3 Graphical presentation of moisture content during vermicomposting

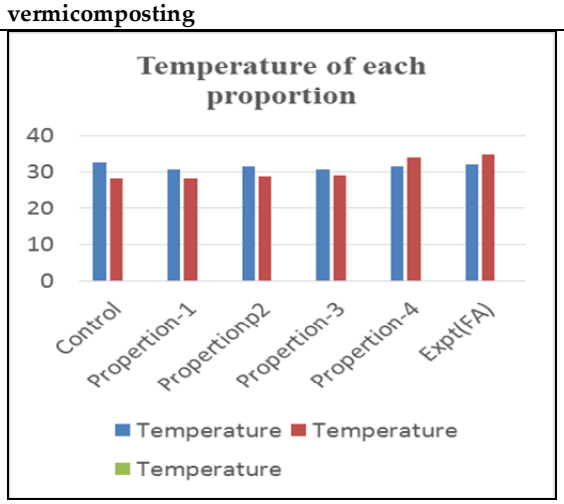

Fig.4 Graphical presentation of Temperature during vermicomposting

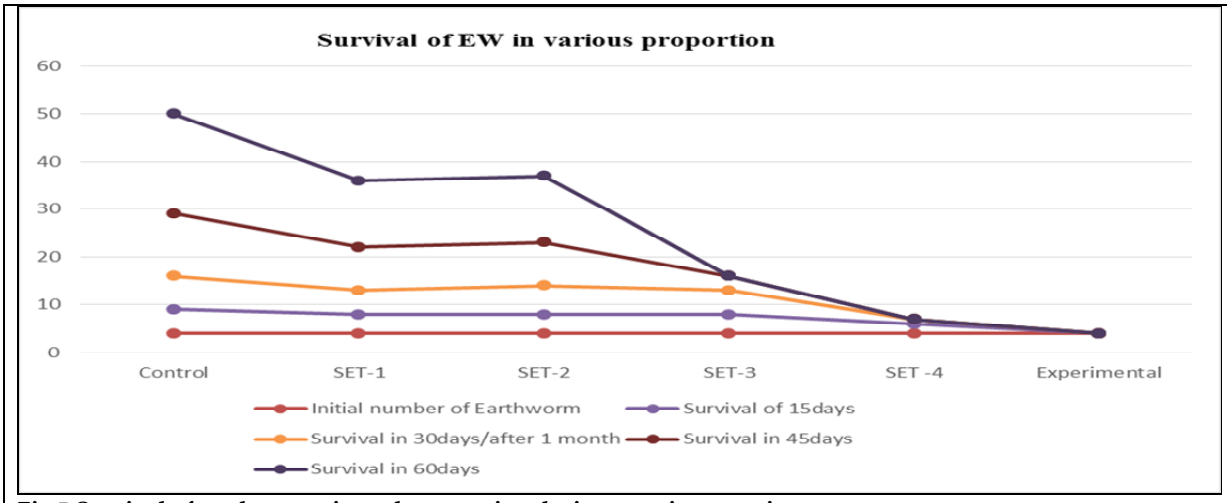

Fig.5 Survival of earthworms in each proportion during vermicomposting

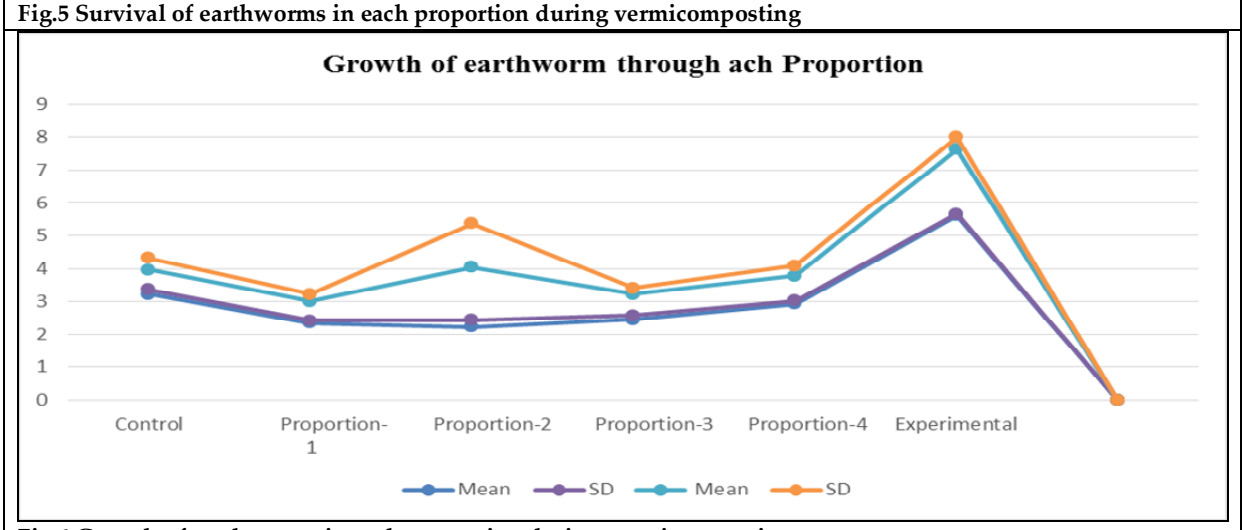

Fig.6 Growth of earthworms in each proportion during vermicomposting

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RESEARCH ARTICLE

Studies on Survival of Tardigrade with Respect to Stress in Temperature of the Most Invincible Micro Animal

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ABSTRACT

Number of organisms present in the living world with special characteristics to survive in any adverse conditions are vital for both environmentally and economically beneficial. The Tardigrades are one of the group of animals popularly known as water bears. Tardigrades survive in lichens and mosses, usually associated with water film on mosses, liverworts. More species are found in milder environments such as meadows, ponds and lakes. These are closely related to Arthropoda and Nematodes based on their morphology. They are the microanimals which can live in extreme conditions. Knowing from literature study about their adaptation, they are quite investigating among the most stress tolerant animals. Experiencing adverse environment conditions, they enter a reversible ametabolic state termed as anhydrobiosis and is known to confer tolerance to a variety of stresses. The present study was conducted to determine the identification and stress tolerance with respect to various temperature of Tardigrades available in locality.

Keywords: water, temperature, microanimals, environment, adaptation.

INTRODUCTION

Tardigrades are among the most resilient animals and have survived exposure to outer space as it withstand large amount radiation, temperatures ranging from 300ºF to near absolute zero and it possibly withstand the pressures of the deepest trenches of the oceans. It can endure extreme temperatures ranging from more than 100ºC down to 196 degrees below zero. They can exposed to 5000grays of radiation and to be just fine while 5 to 10 grays are fatal to human. Recently scientists studied the genome to find out the mechanism by which they are so tolerant to radiation.

Their greatest adaptation that permits them to live in a habitat to dry slowly and go into a dormant state (a kind of behavioral/physiological adaptation). A colorful photo of a tardigrade, popularly known as a "water bear," has won a top prize in the first-ever Olympus Global Image of the Year Award that was created to honor the best life science microscopy images in 2019. (Fig:1).The objective of present study are the identification of tardigrades from moss as well as from lichen and study it's survivability in summer season, rainy season and in winter season.

MATERIALS AND METHODS

Study Area

The present experiment was carried out in Department of Zoology, CUTM campus, Odisha, India.
Kingdom: Animalia
Scientific name: Tardigrade
Phylum: Tardigrada
Super phylum: Ecdysozoa
Rank: Phylum

Collection of Materials

Mosses and lichens selected for this experimental study were collected from Centurion University of Technology and Management, BBSR, Odisha, India and some sample was also collected from eastern area of Bhubaneswar during rainy and winter season. The sample of moss leafy green stuff was collected from wall of boundaries, buildings, trunk of mango trees etc.by srapping from CUTM and the lichen of different colours were collected from eastern area of Bhubaneswar ,Odisha, India they may all have different diversities of tardigrades.

Sampling and Extraction of Experimental Micro animal

The collected lichens and moss were brought to the lab and kept in different petridishes. The leaf of moss and lichen was minutely segregate for extraction of microanimal and allowed to experiment in various treat of temperature. The collected moss and lichen were allowed to soak in water with respect to maintain in various temperature such as boiling, hot , warm, normal ,cold and freeze.The moss sample was soaked overnight (24 hours) in a bowl which was scrapped off and then finally the debris pipetted from the bottom of soaked bowl and a small amount of moss is taken in a slide to observe microanimal tardigrade under light microscope with setting of 5x objective ,10x eye piece ,40x magnification. For this experiment moss containing naturally desiccated tardigrades was used. 0.5 g of dry moss. Moss was slowly hydrated at room temperature and collected tardigrades from their substrate.

RESULT

Tardigrades were collected from CUTM campus and eastern area, Bhubaneswar,Odisha in summer (May),rainy season (August) and in winter season (December)from moss and lichen.

Survivability Rate:

1.After exposure to low temperature (cryobiosis) freezing at -18 degree celcius (approx) in freezer,the microanimal formed as tun.
2. In salt solution (osmobiosis) tardigrade was turned to tun.
3. Response of desiccated tardigrades after heat stress at 37°C
4. A mean of 25.8 (s.d.=6.6) tardigrades have been extracted from moss and a mean of 24.5 (s.d.=7.2) animals have been extracted.

From the present study it was observed that the tardigrates were having survivability after exposure to low temperature (cryobiosis) freezing at -18 degree celcius (approx in freezer, the microanimal formed as tun, moderate and also in high temperature. The salinity taste was also proven as the earlier record that the locality tardigrate was turned to tun in salt solution (osmobiosis).

DISCUSSION

In both experiments, the tardigrades is in cryptobiotic state that is cryobiosis and osmobiosis. In cryobiosis the temperature decreases and water in the cell has frozen, molecular mobility stops permitting the tardigrade to survive in low temperature and it formed as tun. if an animal is viable or dead can be problematic with tardigrades as they tend to become passive under unfavorable conditions such as asphyxia. In an attempt to avoid unfavorable conditions and maintain a somewhat identical post experimental environment, the animals were regularly supplied with clean water and using a Pasteur pipette oxygen was "bubbled" into the water to avoid low oxygen levels. Fundamentally two conditions can be recognized dead or living, though the living can be subdivided into two sub conditions. A major problem during the post experimental observation period was an inevitable fungal infestation and the massive propagation of their hyphae, sometimes covering everything in the embryo dishes. To diminish effect on mortality the fungi had to be removed, or "weeded" out, as often as possible

CONCLUSION

The animals of the phylum Tardigrada remain a little-known, little-studied group despite their overall abundance. Its survivability condition in exposure to freezing that is cryobiosis a form of cryptobiosis, when the temperature decreases and water in the cell has frozen .The result of inhibition of molecular mobility is tun where tardigrade survive for decade. Its survivability condition in salt solution that is osmobiosis that permits tardigrade to tolerate high salinity and form a tun, but tardigrades have already high salt. At the same time, tardigrades present a unique opportunity for research. They are easy to work with, forgiving about collection, and their removal does little environmental damage.They have been applied in transplantology because of their cryptobiotic effect. Though there are studies emphasizing on their survivability importances is a need for more research to understand their relevance in different fields of science.

REFERENCES

1. Acta Zool. Lilloana 38(1): 45-50. Collins, M. and Bateman, L. 2001. The ecological distribution of tardigrades in Newfoundland. Zool. Anz. 240: 291-297.
2. Bertolani, R. 1983. Tardigardi muscicoli delle dune costiere Italiane, con descrizione di una nuova specie. Atti Soc. Tosc. Sci. Nat. Mem., Ser. B 90: 139-148.
3. Bertolani, R. 2001. Evolution of the reproductive mechanisms in tardigrades – a review. Zool. Anz. 240: 247-252.
4. Bertolani, R. and Biserov, V. I. 1996. Leg and claw adaptations in soil tardigrades, with erection of two new genera of Eutardigrada, Macrobiotidae: Pseudohexapodibus and Xerobiotus. Invert. Biol. 115: 299-304.
5. Bertolani, R. and Rebecchi, L. 1996. The tardigrades of Emilia (Italy). II. Monte Rondinaio. A multihabitat study on a highaltitude valley of the northern Apennines. Zool. J. Linn. Soc.116: 3-12.
6. Bertolani, R., Guidetti, R., Jönsson, K. I., Altiero, T., Boschini, D., and Rebecchi, L. 2004. Experiences on dormancy in tardigrades. J. Limnol. 63: 16-25.
7. Bertolani, R., Rebecchi, L., and Beccaccioli, G. 1990. Dispersal of Ramazzottius and other tardigrades in relation to type of reproduction. Invert. Repro. Devel. Rehovot 18(3): 153-157.

8. Binda, M. G. 1984. Notizie sui tardigradi dell'Africa Meridionale con descrizione di una nuova specie di Apodibius(Eutardigrada). [Remarks on some species of tardigrades from Southern Africa and description of Apodibius nuntius n. sp.]. Animalia 11(1-3): 5-15.
9. Boeckner, M., Collins, M., Finney-Crawley, J., and Bateman, L. 2006. The bryofauna of remote coastal Labrador: Including a review of current Canadian records. Zootaxa 1105: 1-16. Bonifacio,
10. Corbet, S. A. and Lan, O. B. 1974. Moss on a roof and what lives in it. J. Biol. Ed. 5: 153-160.
11. Crowe, J. H. 1972. Evaporative water loss by tardigrades under controlled relative humidities. Biol. Bull. 142: 407-416.
12. M. C. and Rossi, G. C. 1984. Contribucion al conocimiento de los tardigrados de Argentina. 4. [Contribution to the knowledge of tardigrades from Argentina. 4.]. Acta Zool. Lilloana 38(1): 45-50.

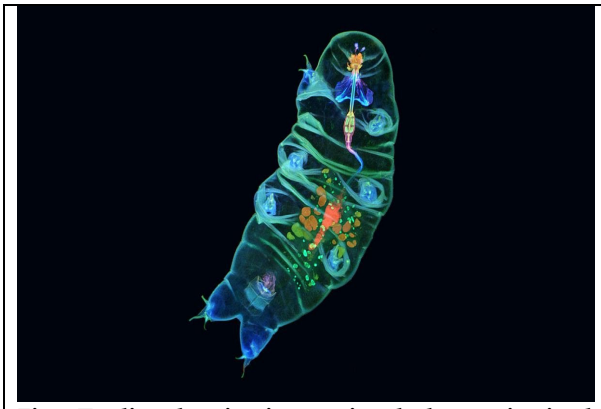

Fig.1 Tardigrade wins international photo prize in the year 2019

Fig.2 Lichen collected from eastern area of Bhubaneswar

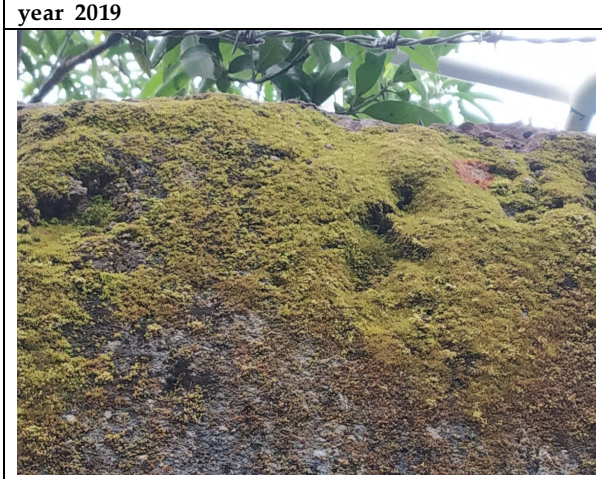

Fig. 3 Moss collected from wall of CUTM campus, Odisha

Fig. 4 Moss collected from wall of building CUTM campus, Odisha

Fig. 5 Moss soaked overnight (24 hours)

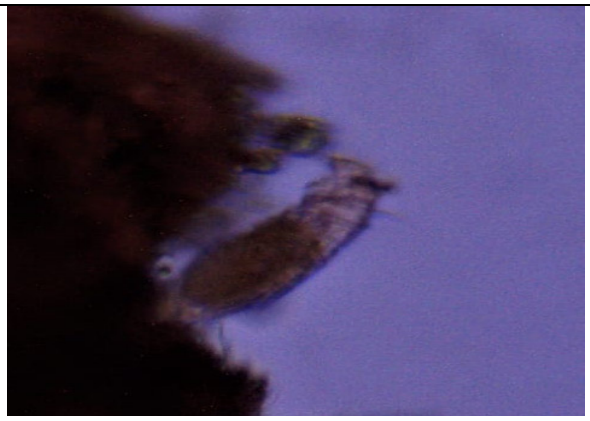

Fig.6 Microanimal tardigrade observed under light microscope in soaked moss

Fig.7 Lichen soaked overnight (24 hours)

Fig.8 Tardigrades observed in soaked Lichen under light microscope

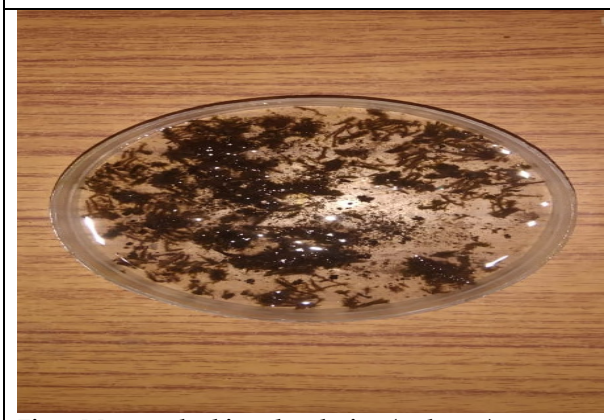

Fig. 9 Moss soaked in salt solution (48 hours)

Fig. 10 Moss after osmobiosis

Fig. 11 Moss exposure to cold temperature

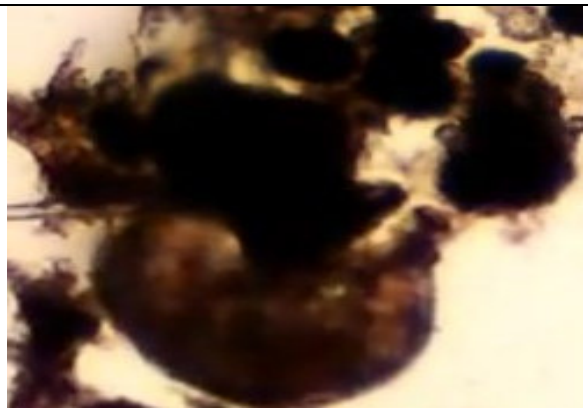

Fig. 12 Formation of Moss (Cryobiosis) (-18 ^{0}C in freezer)

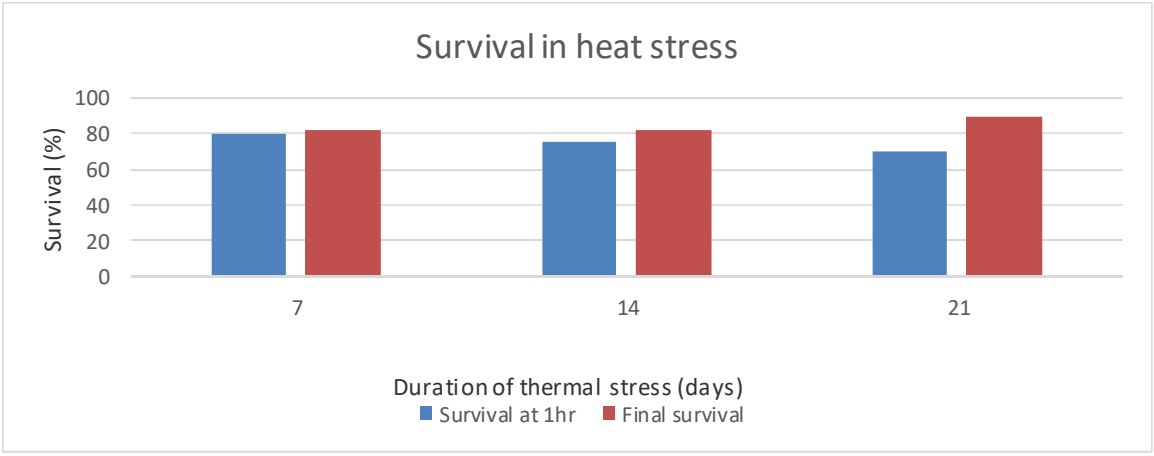

Fig.13 Survival of desiccated specimen after heat stress at 37 degree Celsius

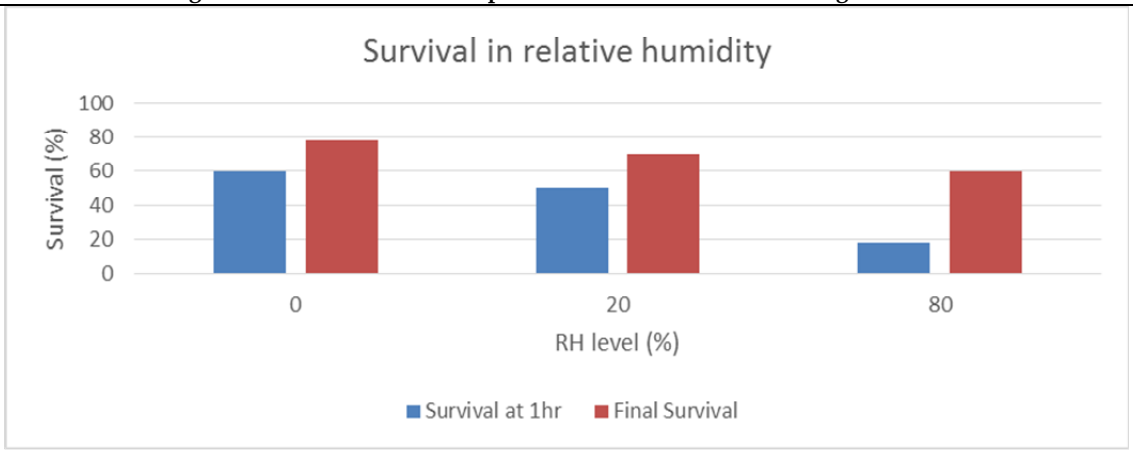

Fig.14 Survival of specimens desiccated within moss and exposed to differrent air relative humidity (RH) and to heat stress at 37 degree celcius for 21 days .

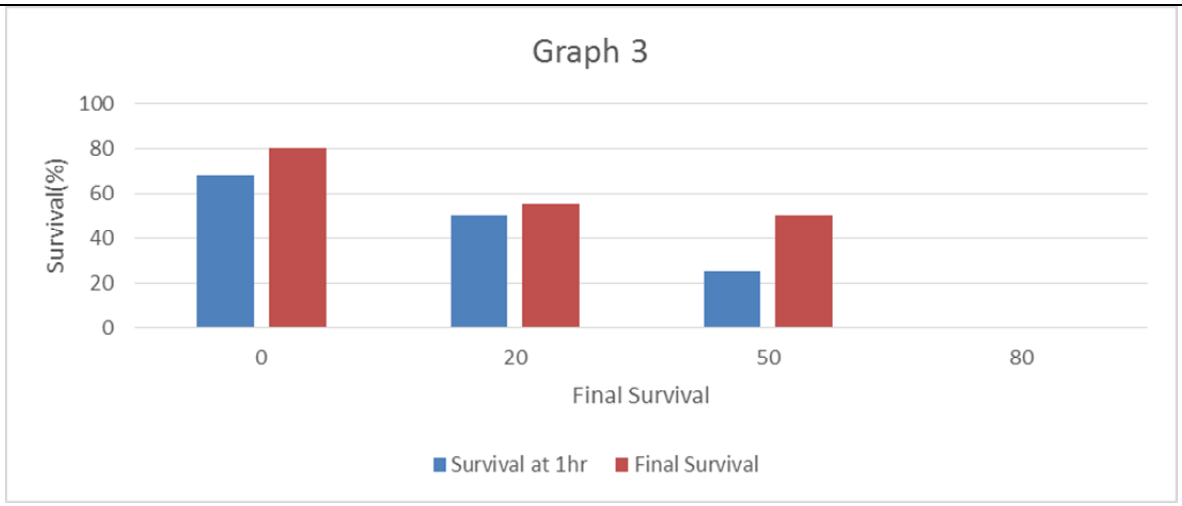

Fig.15 Survival of specimens experimentally desiccated on blotting paper and exposed different values of air relative humidity and to heat stress at 37 degree celcius for 21days

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RESEARCH ARTICLE

Morphological Studies for Identification of Verm: *Eisenia foetida*- A Biological Manipulator

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ABSTRACT

Earthworms are play a vital role in soil ecosystem and an indicator of soil quality. It also acts as bio-manipulator. So that earthworms are also called as farmer's friend or biological indicators or else referred as ecosystem engineers. They play a crucial role in maintaining soil productivity. Their burrowing, feeding, and casting activities alter the physical, chemical, and biological properties of soil. Their activity is response according to morphological and anatomical features. The present study was conducted to identify the morphological features that occurred in *Eisenia foetida* which differs from others to play in vermicomposting. The earthworm species *Eisenia foetida* collected from azola tank used for vermiculture in composting unit at Centurion University of Technology & Management, Bhubaneswar, Odisha, India. The statistical result analysis showed that the selected earthworm identified based on the morphometric parameters but not on soil type that resembles to*Eisenia foetida*.

Keywords: Clitellum, Vermicomposting, *Eisenia foetida*,Morphological features

INTRODUCTION

In ecosystem earthworms play a major role in soil mechanism and conversion of organic waste into manure for sustainable production of crop. The earthworm species found throughout the globe are mostly responsible for enhancing soil fertility but some of the special types are contributed for degradable of waste into manure. The *Eisenia foetida*is one of the composting worm or verm occurs all over the world but mostly in Europe regions (Savigny, 1826) commonly referred to as the tiger worm, redwiggler worm. It is currently be largely found in in India, Uganda and Myanmar of all continental region (except antractica continental region) and also UK,USA and France. It ranges in

size from about in "60 -115 mm length to huge specimens of over 115 mm". The segments in *Eisenia foetida* fluctuateswith a thick cylindrical collar – the clitellum between 5 – 7segments. It has a red brownish sheen and the subsequent segments are consistently elongated to a point. It also described as uniformly pigmented worm (Blackburn 1989). There is a great taxonomic diversity of Eisenia – to which *Eisenia foetida* belongs(Savigny, 1826) . This study aims to test for phenotypic differences within earthworm numerical measurements. The earthworms were sampled in azola tank Centurion University,Bhubaneswar campus location. It is having 3 separate clusters may characterize different families within the earthworm – *Eisenia foetida*. (Savigny, 1826) (ref. ID; 6036, 6916, 6947).It is hugely used in the conversion of organic wastes by using a technique vermicomposting.

MATERIAL AND METHODS

A mapping of composting site was helpful to spot samples of earthworm and for identifying different habitats of sample. New records have been previously sampled which useful to get different results for the present study. Sample was collected by taking proper permission for sampling which must be required for field work assessment. The sample of earthworm was collected by digging a soil pit and removed the contents using a small spade. The required species was collected from azola tank(composting unit) is situated in CUTM campus,BBSR, Odisha, India in 10ft × 8ft × 5ft concrete tank .Then collected species was washed and cleaned in running tap water. Only adult earthworms that were found in the soil was collected in a plastic container. The soil was returned to the pit once the contents has been sorted. Sexually mature earthworm was determined by the presence of the clitellum. Ten specimens were collected from study site and preserved. Morphometric studies of *Eisenia foetida* from azola tank populations was estimated length and and diameter. The body weight is nearly 0.02gm then collected specimen was preserved for calculating of annulus and anatomical study correlate to morphological characters help in identification process.

RESULT

From the present study the characteristic of *Eisenia foetida*were determined by it's "colour and position of clitellum and soil types". The colour were are appeared very deep red in "colour at the anterior (head)" end and "lighter brownish at the posterior (tail)" end. These earthworms were mixed with cow dung and as presented. It was observed that earthworms from Centurion University, BBSR Campus was habitat with clay/loam soil. According to earthworm identification feature. From the table, it is seen that, Earthworms from no.1 and 6 has the utmost body size diameter of 0.7cm and 1cm respectively and earthworm no.6 and 1 with body volume of 6.28 cm^3 and 3.51cm^3 .However, earthworms from no.6 and 10 had the highest values for body weight like 1.12 gm and 0.98 gm. The earthworm with the highest number of segments was 115 those from no. 6 while those from no.8 had the lowest number of 60 segments. Very small in size according any other species type found in earthworm. Male pores in 9^{th} at or somewhat below clitellum each at the lateral end of a deep transverse cleft. Tubercula pubertates stretch along the ventral border of the clitellum over 3th to 5th segments is uniformly pigmented in nature. Pale or dark coloured near the genital pore. Reddish brown colour with golden shade saddle or pillion shaped clitellum covers 4-9 segment. The mean length of 50 -130 mm,a diameter of 3-6 mm and a segment number varying between 60 -115. Single species recorded in India and also its subcontinent region also probably found in Paris, France, UK and USA. It can survive, grow and reproduce in temperature ranges from 15-270C,moisture content ranges42-85%and pH level with 6-8.2 as per experimentally observed.(int-source-bioweb.uwlax.edu).This ability to adapt wider ranges of environmental conditions of the species made it used for vermicomposting. From this study it was carefully monitored and statistically analyzed certain characteristics of the collected species that identified as *Eisenia foetida*resembles approximately with the characteristics that reported from literatures (Silvia M.,et al. ,2009) and simplified key to common genera of terrestrial earthworm with following characters

Domain – Eukarya(true nucleus with membrane bound organelles)
Kingdom- Animalia(Multicllular,heterotrophic)
Phylum – Annelida(Annules present throughout entire body)
Class - Oligochaetae (Setae located ventrally, laterally or dorsolaterally,hermaphrodite)
Order - Heplotaxida (Male pore at 4-7 segments)
Family - Lumbricidae (Sadle shaped clitellium ranges-9-12 segments, Gizzard at 17-19 segments)
Genus - Eisenia (According to G.Eisen's name,1900-reported)
Species - *Eisenia foetida* (Savigny,1826)-
(foetida means foul smelling produced from it's body when unfavorably handled)

CONCLUSION

In the present investigation the collected species were studied based on body size characters, thus differences in clustering could be attributed to the body size measurements across locations. Sims and Gerard (1985) suggested that the environments inhabited by most earthworms were quite stable and these determined the time it takes to mature in some species. Also *Eisenia* earthworms divided into 2 distinct categories – the 'r' and 'k' selected species based on their body sizes and lifestyles. The 'r' selected species usually had small body sizes, shorter incubation and maturation times and in habited stable surface environments. The k-selected species however had large body sizes, and in habited stable environments. Even though the age of these earthworms were not determined in the study, they were all sexually mature at the time of collection as shown by the presence of the clitellum. Collections of no.8 specimen fromazola tank had small body sizes and were from mixture of cow dung and clay or loamy soil, thus having some relationship with r-selected species. Earthworms -no.6 usually contains large amounts of decaying plant materials like leaf and bark which when used as food by the earthworms may have contributed to their large body sizes.

REFERENCES

1. Blackburn, J.C. 1989. External anatomy of earthworms. Sci. 207: 2572 – 2577.
2. Chaudhuri PS, Pal K, Bhattacharjee G and Dey SK (2002). Chemical changes during vermicomposting (Perionyx excavatus) of kitchen wastes. Trop.Ecol41: 107-110.
3. Darwin CR (1881). The formation of vegetable mould through the action of worms with observation on their habits. Murray, London.
4. Edward CA and Neuhauser EF (1988) Earthworms in waste and environmental management.
5. Edwards CA. and Boglen PJ (1996). Biology and Ecology of earthworms, 3rd Edition, Chapman and Hall publication, 2-6 Boundary Row London, UK, 202-217.
6. Gregory, T.R. and P.D.N. Herbert. 2002. Genome size estimates for some oligochaete annelids. Can. J. Zool. 80: 1485 – 1489.
7. Heethoff, M., K. Etzold and S. Scheu. 2003. Mitochondrial C011 sequences indicate that the parthenogenetic earthworms Octolasion tyrtaeum (Savigny 1826) constitutes of two lineages differing in body size and genotype. Pedobiologia. 47: 9 – 13.
8. Lavelle, P. 1988. Earthworm activities and the soil system. Biol. Fert. Soils. 6: 237 – 251.
9. Nadia Zeguerrou & Rachid Adjroudi & Abdelkrim Si Bachir & Mohamed El Hadef El Okki, 2019. "Assessment of ammonium hydroxide effect on Eisenia fetida (Savigny, 1826): acute toxicity and avoidance tests," International Journal of Agricultural Resources, Governance and Ecology, Inderscience Enterprises Ltd, vol. 15(1), pages 27-44.
10. Pirrone, S. 1985. The earthworm baits market in North America. Heredity. 59: 1019 – 1029. 20 Nature and Science, 5(2), 2007, B.O. Oboh, D.O. Akintobi and C. Ejidereonwu, Morphometric studies in Eudrilus eugeniae populations from different locations in Lagos, Nigeria 21

11. Rodriguez, A.C. and I.R. Lapeire. 1992. Increase in weight, length and number of segments of Eudrilus eugeniae (Oligochaeta: Eudrilidae) at 240 C. Rev. Biol. 6: 215 – 221.
12. Segun, A.O. 1998. Tropical Zoology 2nd edition. University Press, Ibadan. 283pp.
13. Shagoti, U.M. 1985. Analysis of developmental rates and body size in earthworms. Heredity. 80: 29 – 40.
14. Sims, R.W. and R. Gerard. 1985. A review of the economic importance of earthworms. Science. 29: 152 – 160.
15. Swofford, D.L. and G.J. Olsen. 1990. Phylogeny Reconstruction P411-501D.M. in Hills and C. Moritz (eds) Molecular Systematic. Sineaur Associates, Sunderland, MA.
16. Terhivuo, J. and A. Saura. 1993. Clonal and morphological variation in marginal populations of the parthenogenetic earthworms Octolasion tyrtaeum and O. cyaneum (Oligochaeta Lumbricidae) from eastern Fennoscandia. Boll. Zool. 60: 87 – 96.
17. Tian, G., L. Brussard and B.T. Kang. 1995. Breakdown of plant residues with contrasting chemical compositions: Effect of earthworms and millipedes. Soil Biol. Biochem. 27: 277 – 280.
18. Tian, G., J.A. Olimah, G.O. Adeoye and B.T. Kangi. 2000. Regeneration of earthworm populations in a degraded soil by natural and planted fallows under humid tropical conditions. Soil. Sci. Soc. of America. J. 64: 222 – 228.
19. Viljoen, S.A. and A.J. Reinecke. 1992. The temperature requirements of epigeic earthworm species Eudrilus eugeniae (Oligochaete); a laboratory study. Soil. Biol. Biochem. 24: 1345 – 1350.
20. Vitturi, R., M. S. Colomba, A. Pirrone and A. Libertini. 2000. Physical mapping of Rdna genes (TTAGGG)n telomeric sequence and other karyological features intwo earthworm of the family Lumbricidae(Annelida: Oligochaeta). Heredity 85: 203-207.
21. Weeks, J.M. and C. Svendsen. 1996. Neutral red retention by lysosomes from earthworm (Lumricus rubellus) coelomocytes: A simple biomarker of exposure to soil copper. Env. Toxicol. Chem. 15: 1801 – 1805.

TABLE- 1 Identification of earthworm Esenia foetida

NO.	Obse	SPECIES	LENG	DIAM-	BODY	BODY	HEA	SPERMATHE	CLITE	BODY
1.	1st	E.fetida	7cm	0.8cm	0.92	3.51	EPI	10^{th} segment	4 to 7	102
2.	2nd	*E.foetida*	4.3cm	0.3cm	0.19	0.3	EPI	10^{th},11^{th}, 12th Segment	4 to 7	74
3.	3rd	*E.foetida*	5.9cm	0.6cm	0.23	1.66	EPI	10^{th},11^{th},12th segment	4 to 7	85
4.	4th	*E.foetida*	6.3cm	0.4cm	0.69	0.79	EPI	10^{th},11^{th},12^{th} segment	4 to 8	89
5.	5th	E.fetida	6.7cm	0.7cm	0.44	2.57	EPI	10^{th},11^{th},12^{th} segment	4 to 7	93
6.	6th	*E.foetida*	8cm	1cm	1.12	6.28	EPI	10^{th},11^{th},12^{th}, 13^{th}segment	4 to 8	115
7.	7th	*E.foetida*	5.3cm	0.6cm	0.57	1.49	EPI	10^{th},11^{th} segment	4 to 8	78
8.	8th	*E.foetida*	4.1cm	0.1cm	0.35	0.03	EPI	9^{th},10^{th} segment	4 to 7	60
9.	9th	*E.foetida*	6.7cm	0.2cm	0.76	0.21	EPI	10^{th},11^{th},12^{th} segment	4 to 7	82

10.	10th	*E.foetida*	7.4cm	0.7cm	0.92	2.84	EPI	11^{th},12^{th},13^{th} segment	4 to 8	109
11.	MEAN	*Morphometric of E.foetida*	6.14	0.58	0.169	1.968		10^{th},11^{th},12^{th}	4 to 7	88.7
12.	SD		1.278	0.302	0.316	1.928				16.71

Fig 1 Measurement and Identification of Morphometric characteristics of *Eisenia foetida*

Fig 2 Measurement and Identification of Morphometric characteristics of *Eisenia foetida*