Journal of the Nigerian Association of Mathematical Physics
Volume **20 (March, 2012), pp 131 – 138**

Modeling the effect of operating variables on sorption of PAHs from aqueous streams onto orange peels using artificial neural network pattern recognition.

****Owabor, C.N. and Issa A.A.***

Department of Chemical Engineering,
University of Benin, Benin City, Nigeria.

Abstract

The application of artificial neural network (ANN) technology to the simulation of factors affecting sorption of polycyclic aromatic hydrocarbon (PAHs) onto ripe and unripe orange peels is presented in this work. A 3-layer backward propagation network structure was applied using pattern recognition tool in MATHLAB 7.9.0 (R2009). Optimum number of neurons in the hidden layer used was 20 with MSE value of 0.000912. Parameters such as contact time, adsorbent dosage, pH, and particle size were used as input variables while the output of the ANN was the pollutant removal concentration.

The study showed that neural network pattern recognition generated data for pollutant removed using ripe and unripe orange peels agreed to a large extent with the laboratory data. The regression correlations obtained for both ripe and unripe orange peels closely approximated to 0.99. In general, the result of this study indicated that particle size was the most significant factor that affects sorption of PAHs. The other factors considered in this study affected the sorption of PAHs in the order, contact time> pH > adsorbent dosage.

Keywords: ANN, Backward propagation, MSE, Effluent concentration, Pollutant removal efficiency.

1.0 Introduction

One of the unit operations used for the treatment of contaminated water is adsorption [1]. The process usually is conducted either as a batch or column study. The latter is aimed at determining the kinetics and isotherm constants while the former is performed for determining the breakthrough curve. The pollutant removal efficiency (PRE) is the most significant output of adsorption studies with respect to wastewater treatment. The variation of PRE depends on several factors such as adsorbent characteristics, contact time, adsorbate concentration, temperature, adsorbent dosage e.t.c [2].

Modeling of the removal of contaminants from waste streams has been conducted over the years using deterministic and probabilistic models [3-5], stochastic models [6] and multiple second-order polynomial regression model [7]. These models have proved to be successful in their predictions. However, in recent years, artificial neural network has become popular as they have been reported differently as attractive [8], efficient [9], more accurate and predictive than the multivariate regression models [10]. ANN can perform a human- like reasoning, learns and stores the relationship. They are simplified models of the biological structure of human brains. A neural network model consists of an interconnected assembly of simple processing elements, neurons, which are organized in layered fashion [11]. Generally, neural network model architecture consists of three main layers: an input layer (independent variables), an output layer (dependent variables) and one or more intermediate hidden layers [12]. It is a collection of mathematical models that emulate the real neural structure of the brain and it is made up of individual interconnected simple processing elements called neurons, arranged in a layered structure to form a network that is capable of performing massive parallel computation. Its architecture is illustrated in Figure 1.

*Corresponding author: ***Owabor, C.N.,*** E-mail: owabor4you@yahoo.com, Tel. +2348034101218

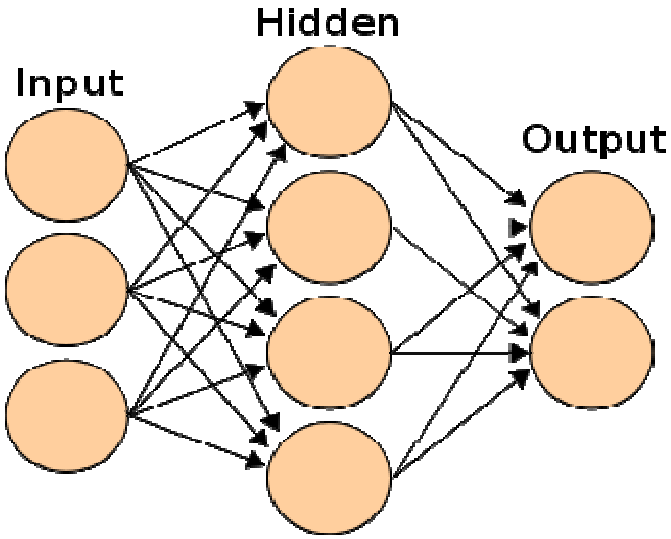

Figure 1: Architecture of artificial neural network

ANN can perform human-like reasoning, learns and stores relationship of the processes on the basis of the available representative data set. By mimicking the network of real neuron in the human brain, ANN performs mapping from an input space to an output space.

Neural networks have been used as a promising technique, when complex reaction systems cannot be well identified, or in the case of lack of basic knowledge of reaction mechanisms. It has been claimed that artificial neural networks are 120–5000 times faster than phenomological models [13]. Artificial neural network and multiple linear and non-linear regressions are among the most widely used stochastic models for predicting effluent pollutant concentration [14-15].

While regression technique is widely used for any physical modeling purposes [16], the report of [17] obtained from the analysis of a compiled database pertaining to adsorption isotherm constants using regression analysis and neural networks further suggests that regression techniques fail to represent the mechanism of adsorption. This was attributed to the fact that the ANN model gives better results for predicting results (output) from adsorption database. They concluded that the conventional analysis using regression technique is not suitable for adsorption experimental data since the technique fails to understand the physics of the system.

Advances in recent times has projected ANN as a fast growing popular choice among engineers and scientists as one of the powerful tools for predicting contamination and concentration of different effluents and chemicals in drinking water, wastewater and aquifers [18-20]. This is hinged on the ability of artificial neural networks to relate the input and output variables without having prior knowledge of the physics of the system. The important operational condition is the availability of an accurate and large amount of data on the system variables to train the networks. The neural networks yield solutions to complex phenomena where the relationships and rules are not known The Back-Propagation Network (BPN) is one of several networks that is widely used for predicting the output and is successfully applied to a wide range of problems [2, 21].

The objective of this study is to compare data on the effects of particle size, adsorbent dosage, contact time, and pH on the sorption of naphthalene onto ripe and unripe orange peels obtained from laboratory experiment with simulated data from neural network pattern recognition tool using backward propagation with known hidden layer.

3.0 Methodology

The following parameters are considered significant in the study of the sorption of PAHs: adsorbent dosage, pH values, contact time, and particle size.

In this study, the data on adsorbent dosage, contact time, pH values and particle size were obtained from literature report on sorption of polycyclic aromatic hydrocarbons onto ripe orange peels [22] and unripe orange peels [23]. MATHLAB 7.9.0 (R2009) software was used to run the simulation. The mathlab runs a three phase simulation which includes

training, validation and testing. The levenberg-marquardt (lm) back-propagation algorithm was used for the training of ANN model.

The trained artificial neural network model was then tested and validated with the experimental results to estimate the factor which most affects the sorption of PAHs unto ripe and unripe orange peels.

3.1 Training

The training phase is carried out using the scaled conjugate back propagation. The essence of this training phase is to classify the inputs according to the target after establishing the relationship between the input data. Training automatically stops when generalization stops improving as indicated by an increase in the mean square error (MSE) of the validation samples

Mean Square Error is the average squared difference between the outputs and targets. Lower values are better. Zero means no error.

3.2 Validation

In this phase after relationships must have been established between the input data and the target during training phase, a validation analysis takes place. These are used to measure network generalization and to halt training when generalization stops.

3.3 Testing

The trained neural network can now be tested with the testing samples and this will give us a sense of how well the network will do when applied to data from the real world. These have no effect on training and so provide an independent measure of network performance during and after training.

4.0 Results and Discussion

4.1 Identification of the optimum number of neurons

The simulation started with 2 neurons in the hidden layer and the MSE value was found to be 11.30. The neurons were then increased to 4 and the MSE reduced to 2.2, further increase in the number of neurons gave a sudden increment in the MSE value. This sudden increment was due to the nature of neural network model in which it is likened to the human neurons. Higher number of neurons was found to be proportional to better accuracy of the ANN prediction. This observation is in agreement with literature reports of [9, 21]. At certain point when there were more neurons than that required the accuracy of the prediction reduces. In this study, optimum number of neurons was obtained to be 20 since it has the minimum value of MSE recorded as 0.000912 and as shown in Figure 2.

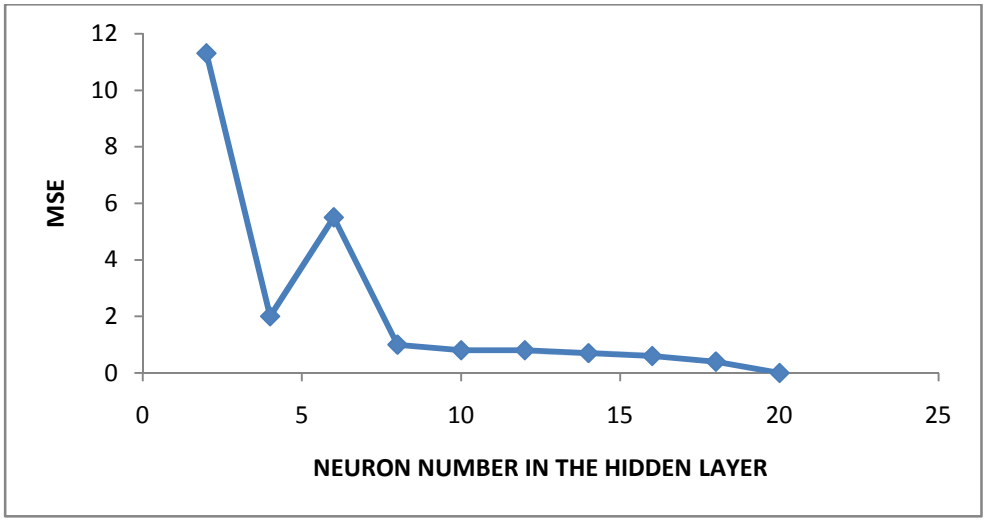

Figure 2: Variation of MSE with number of neurons

4.2 Simulated results for ripe and unripe peels using the ANN

The artificial neural network generated data was obtained for ripe and unripe orange peels with ANN generated expression 3 and 4 respectively with ranking coefficient of 0.9997 and 0.99796 respectively. These ranking correlations show the accuracy of using ANN pattern recognition to predict pollutant removal concentration since it has a very high value of MSE close to unity. This high level of accuracy of neural network makes it a good alternative instead of using other traditional models like regression. The values obtained from this study indicate that there is negligible difference in the accuracy of the predictions of ANN for both peel types.

ANN has become a popular choice among engineers and scientists as one of the powerful tools for predicting pollutant removal because ANNs have the ability to relate the input and output variables without having knowledge on the physics of the system, provided an accurate and large amount of data on the system variables to train the networks is available. The observed output pattern of ANN in this study is consistent with literature report of [10, 21, 24].

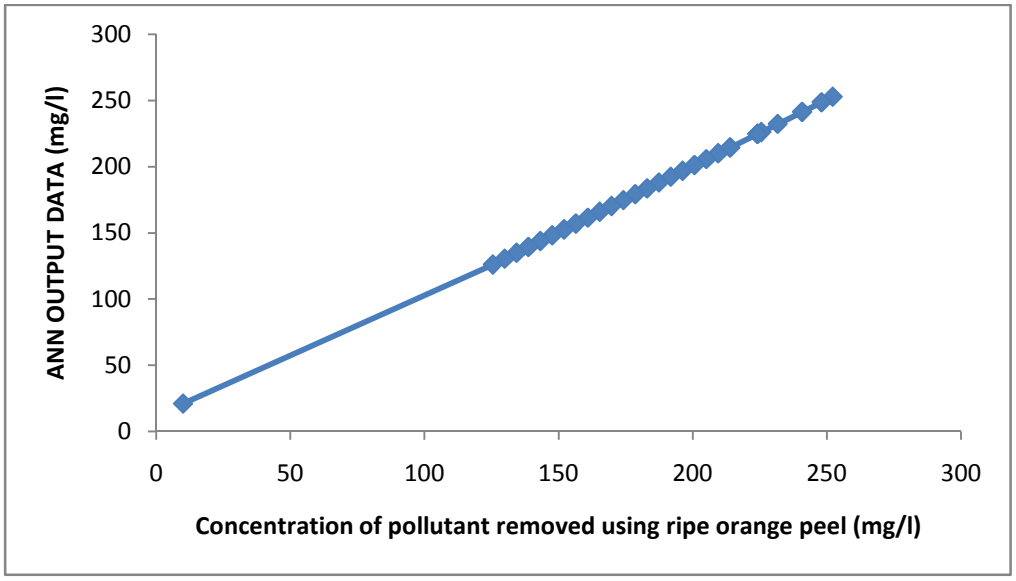

Figure 3: Variation of laboratory data with ANN generated output for ripe orange peel.

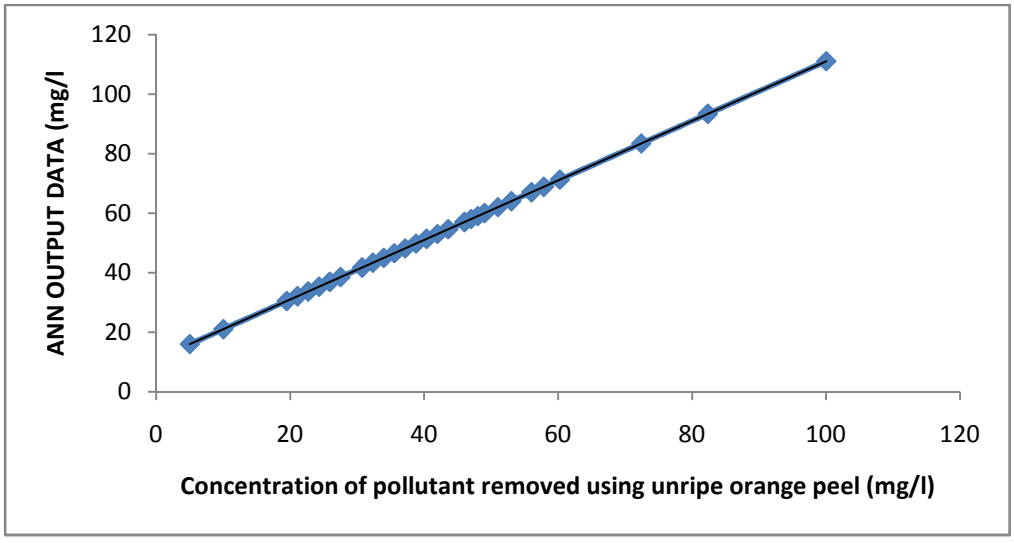

Figure 4: Variation of laboratory data with ANN generated output for unripe orange peel.

4.3 Comparative studies on factors affecting sorption of PAHs onto ripe and unripe orange peel

4.3.1 Effect of adsorbent dosage on pollutant removed onto ripe and unripe orange peels.

For 1mg of both ripe and unripe peels, the concentrations of pollutant removed were 250 and 50mg/l respectively. For every coresonmding increment in the adsorbent dosages, the concentrationm removed onto ripe orange peel were greater than thant removed onto unripe peels.

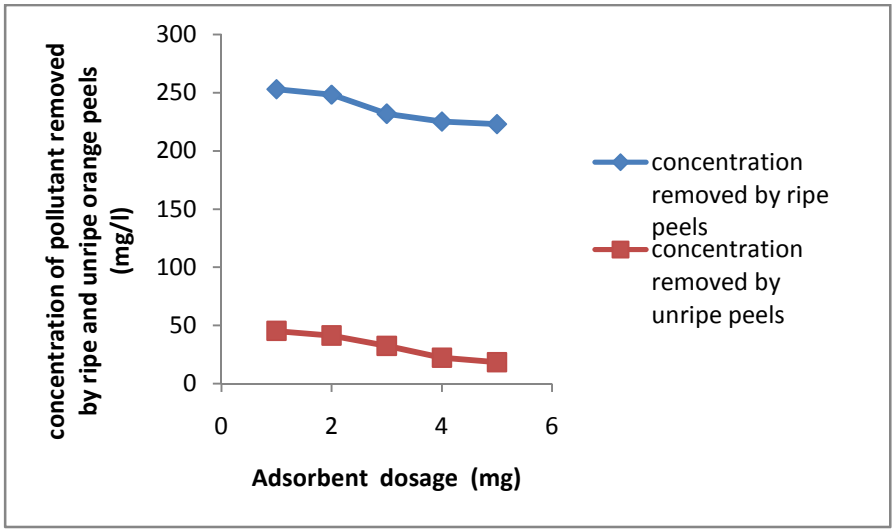

Figure 5: Variation of concentration removed with adsorbent dosage

4.3.2 Effect of pH on pollutant removed onto ripe and unripe orange peels

For pH value of 1.18 on both ripe and unripe peels, the concentrations of pollutant removed were 32.52 and 56.1 mg/l respectively. For coresponding increment in the pH, values from acidic region to the alkaline medium the concentration removed onto ripe orange peel were greater than that removed onto unripe peels. However, concentration of pollutant removed reduced for both ripe and unripe orange peels.

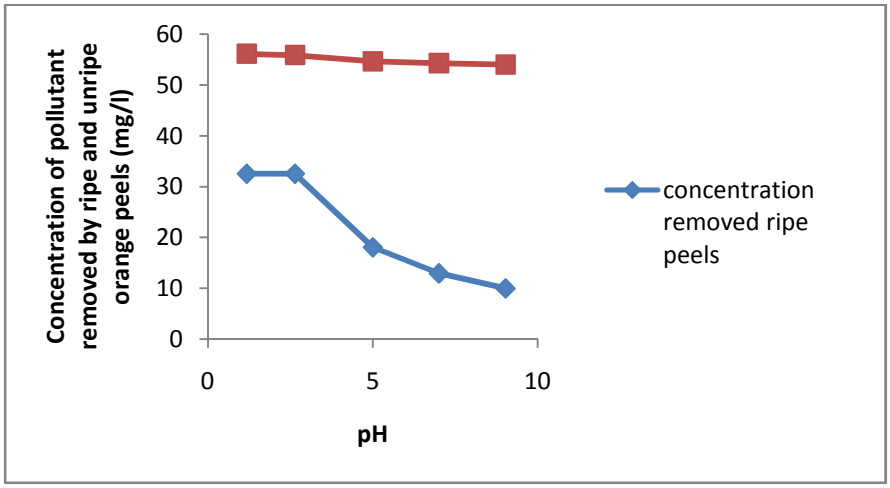

Figure 6 Variation of concentration removed with pH

4.3.3 Effects of contact time on pollutant removed onto ripe and unripe orange peels

Initially, the concentrations of pollutant removed were 250 and 100 mg/l for both ripe and unripe orange peels respectively. For coresponding increment in the contact time, the concentration removed onto ripe orange peel were greater than that removed onto unripe peels. However, concentration of pollutant removed reduced for both ripe and unripe orange peels

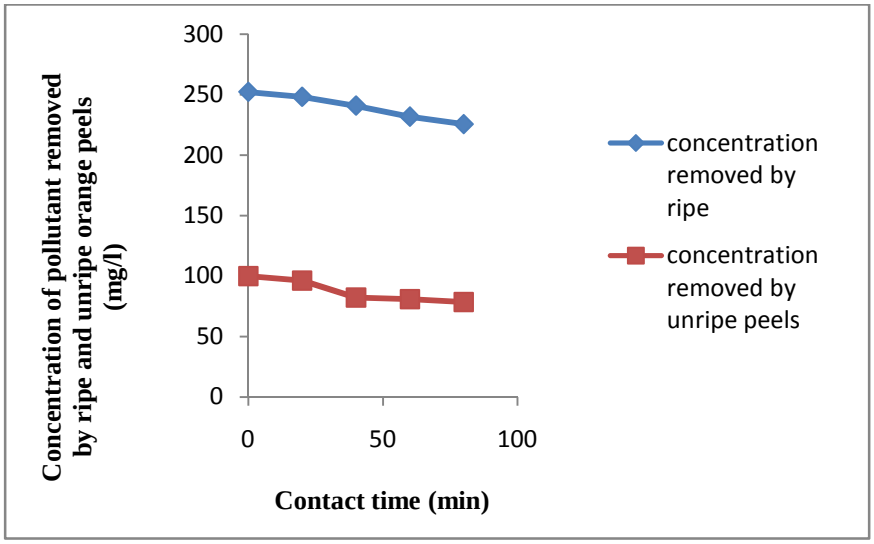

Figure 7 Variation of concentration removed with contact time

4.3.4 Effect of particle size on pollutant removed onto ripe and unripe peels

For particle size of 0.075mm using ripe and unripe orange peels, the concentration of pollutant removed were 9.625 and 24.63 mg/l. increasing the particle sizes, gave increment in concentration of pollutant removed correspondingly onto ripe and unrie orange peels.Nevertheless, concentration of pollutant removed increases for both ripe and unripe orange peels. Further study was carried out on factors affecting sorption of PAHs onto ripe and unripe orange peels as shown in Figures 5, 6, 7 and 8. From this study, it was found that ripe orange peels can be suitably used for adsorbent in the removal of contaminants in aqueous solution as compared to the unripe orange peels.

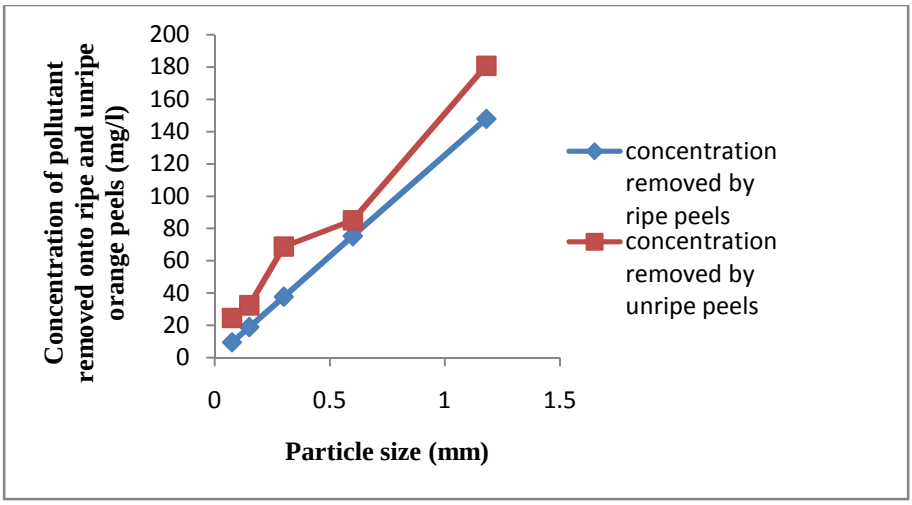

Figure 8 Variation of concentration removed with particle size.

Conclusion

In this present study, a three layer ANN with a tangent sigmoid transfer function at hidden layer and a linear transfer function at output layer were used to predict the concentration of pollutant removed. The architecture of the ANN model had a 4-20-1 network trained with Levenberg-Marquardt (LM) back propagation algorithm. There was a close agreement between the predictions by ANN and the experimental values. The study thus affirms that ANN provides a suitable alternative for the prediction of the concentration of contaminant solute removed from aqueous streams.

References

1. H. Peavy, L. Rowe and G. Tchobanoglous, (1995). Environmental Engineering, McGraw Hill International editions, Singapore.
2. B.V. Babu, V. Ramakrishna and K. Chakravathy. (2000). "Artificial neural network for modeling of adsorption." Birla Institute of Technology and Science, Pilani Rajasthan (India)-333031.
3. M.H. Rahman, N.M. Wasiuddin. and M.R. Islam. (2004). "Experimental and numerical modeling studies of arsenic removal with wood ash from aqueous streams." Canadian Journal of Chemical Engineering, 82 (5), 968-977.
4. E. Smith and K. Ghiassi. (2006). "Chromate removal by an iron sorbent: mechanism and modelling." Water Environment Research, 78 (1), 84-93.
5. R.P. Singh, F. Zahra, W. Savio and S.C. Prasad. (2009). "Axial dispersion and mass transfer controlled simulation study of chromium (vi) adsorption onto tree leaves and activated carbon. Journal of Environmental Engineering, Vol.135, Isuue 10, 1071-1083.
6. A.P.C. Cuco, A.J.S. Neto, H.F.C.Velho and F.L. Sousa. (2009). Solution of an inverse adsorption problem with an epidemic genetic algorithm and the generalized extremal optimization algorith. Inverse problems in Science and Engineering, 17, 289-302.
7. J.F. Fu, Y.Q. Zhao, M. Razali and M. Bruen. (2008). "Response surface optimization of phosphorus species adsorption onto powdered alum sludge." Journal of Environmental Science and Health Part A, 43, 1100-1107.
8. B. Meenakhsipriya, K. Saravanan and S. Sathiyavathi. (2009). "Neural based ph system in effluent treatment process." Modern Applied Science, Vol.3, No.4, 166-176.
9. A.B. Chelani, C.V. Chilapati-Rao, K.M. Phadke and M.Z. Hasan. (2004). "Prediction of sulphur dioxide concentration using artificial neural network." Environmental Modeling & Software 17, 161-168.
10. A.L. Forrest, K.P. Fattah, D.S. Mavinic and F.A. Koch. (2007). "Application of artificial neural networks to effluent phosphate prediction in struvite recovery." J. Environ. Eng. Sci. 6(6), 713-725.
11. O. Gunadym. (2009). "Estimation of soil compaction parameters by using statiscal analyses and artificial neural networks." Environ. Geol, 57, 203-215.
12. T. Khanna. (1990). Foundations of Neural Networks, Addison-Wesley Publishing Company, California.
13. A.L. Tarca, P.A. Bernard and F. Larachi (2003). R einforcing the phenomenological consistency in artificial neural network modeling of multiphase reactors." Chem. Eng. Process, 42 (8-9), 653-662.
14. G.H. Xiu and P. Li. (2000). "Prediction of Breakthrough Curve for Adsorption of Lead(ii) on Activated Carbon Fibres in a Fixed Bed." Carbon, 37, 975-981.
15. K. Yetilmezsey and S. Demirel. (2008). "Artificial Neural Network (ANN) approach for Modeling of Pb(ii) adsorption from aqueous solution by Antep pistachio (Pistacia Vera L.) Shells." Journal of Hazardous Materials, 153, 1288-1300.
16. B.V. Babu and S. Gupta. (2000). "Modeling and Simulation for Dynamics of Packed Bed Adsorption." Proceedings of Intrnational Symposium and 57th Annual Session of IIChE (CHEMCON-2004), Mumbai, December 27-30, 2004.
17. B.V. Babu and V. Ramakrishna. (2003). "Applicability of Regression Technique for Physical Modeling: A case study on Adsorption in Wastewater Treatment." *Proceedings of International Symposium & 55th Annual Session of IIChE (CHEMCON-2002)*, Osmania University, Hyderabad, December 19-22, 2002.
18. A.K. Jain and D. Chalisgaonkar. (2000). "Setting up stage discharge relationship using ANN". J. Hydrol. Eng., 5(4), 428-433.
19. G.U. de Souza, M.A. Selene, L.C. Peruzzo, A.A. Ulson de Souza. (2007). "Numerical study of the adsorption of dyes in textile effluents." Appl. Math. Modell. doi:10.1016/j.apm.2007.06.007.
20. M. Mortula and R. Sadiq. (2009). Application of Artificial Neural Network in Modeling Water Treatment Processes." Proceedings of the Third International Conference on Modeling, Simulation and Applied Optimization, Sharjah, U.A.E January 20-22.

21. C.N. Owabor and B.V. Ayodele. (2011). "Predicting the biodegradation of polycyclic aromatic hydrocarbons (PAHs) in continuous stirred tank reactor by artificial neural network." Journal of the Nigerian Association of Mathematical Physics, Vol.19 (November), 395-398.
22. C.N. Owabor and J.E. Audu. (2010). "Studies on the sorption of naphthalene and pyrene from aqueous medium using ripe orange peels as adsorbent." Global Journal of Pure and Applied Sciences. Vol.16, No 1, 131-139.
23. C.N. Owabor, S.E. Agarry and D. Jato. (2011). "Removal of naphthalene from aqueous medium using unripe orange peels as adsorbent: Effecting of operating variables." Advances in Chemical Engineering Science (in press).
24. X. Du, Q. Yuan, J. Zhao and Y. Li. (2007). "Comparison of general rate model with a new model-artificial neural network model in describing chromatographic kinetics of solanesol adsorption in packed column by macroporous resins." Journal of Chromatography A, 1145, 165-174.