INTERNATIONAL JOURNAL OF ENGINEERING AND MANAGEMENT SCIENCES

www.scienceandnature.org

MODELING PHENOL ADSORPTION IN WATER ENVIRONMENT USING ARTIFICIAL NEURAL NETWORK

Kundu Snigdha
Department of Geology, National Institute of Technology, Durgapur-713209, India

ABSTRACT
In the present work removal of phenol from aqueous solution using peat soil as adsorbent dose was studied. The initial phenol concentration was varied from 5 mg/L to 20 mg/L with varying amount of peat soil (5-20 gm) in laboratory batch adsorption experiment. The maximum adsorption efficiency was found at initial phenol concentration of 10 mg/L, adsorption dose of 200 g/L and pH of the solution of 6.0. The equilibrium contact time was found at 6 hour. A three layer feed forward artificial neural network (ANN) with back propagation training algorithm was developed to model the adsorption process of phenol in aqueous solution using peat soil as adsorbent. The neural network architecture consisted of tangent sigmoid transfer function (tansig) at hidden layer with 20 hidden neurons, linear transfer function (purelin) at output layer and Lavenberg-Marquardt (LM) backpropagation training algorithm. The neural network model predicted values are found in close agreement with the batch experiment result with correlation coefficient (R) of 0.993 and mean squared error (MSE) 0.00105996.

KEYWORDS: adsorption, peat soil, phenol, neural network, correlation coefficient.

INTRODUCTION

Phenol is listed as priority pollutant by United State Environmental Protection Agency (USEPA). The major sources of phenolic waste are petroleum refineries, petrochemical, steel mills, coke-oven plants, coal gas, synthetic resins, pharmaceuticals, paints, plywood industries and mine discharge [1]. Phenol may enter underground or surface waters due to spills from the industries or industrial products and people may be exposed to the chemical by drinking the polluted water or during the utilization of the water for other purposes [2]. The exposure to the phenol can cause serious health problems to the human beings including diarrhea, dark urine and hemolytic anemia [3].

Several methods have so far been proposed for removal of phenol, e.g., biological oxidation, thermal liquid phase oxidation, photochemical conversion, catalytic oxidation, physical adsorption and solvent extraction system [4]. Among all of the methods, low cost physical adsorption process appears to be most effective in removal of phenol from aqueous solutions containing moderate or low concentrations. Investigation had already been carried out for removal of phenol from aqueous solutions by low cost adsorbents such as saw dust [5,6], charcol [7], activated carbon, bagasse ash and wood charcol [8], peat, fly ash and bentonite [9].

In recent years ANN has become a popular choice among engineers and scientists as one of powerful tools for predicting contamination and concentration of different effluents and chemicals in drinking water, wastewater and aquifers. [10]. Various researchers used the ANN for exhibit the performance of adsorption system successfully [11,12,13].

The objective of this work to study the performance of peat soil for phenol removal from industrial wastewater. The artificial neural network model was also developed to study the adsorption process and the accuracy of the model was tested using correlation coefficient, mean squared error (%) etc.

MATERIALS AND METHODS:

Preparation of adsorbent and synthetic phenol solution:
Peat soil used as adsorbent in the laboratory batch experiment was collected the benthos of a nearby pond in Mankar, Dist. Burdwan, West Bengal, India. The soil was dried in hot air oven for 24 hours at a temperature of 100°C.Soil lumps were then crushed by hammer and various physical properties was determined as per Bureau of Indian Standard(BIS). The physical properties of soil are shown in Table.1.

Table 1 Physical Properties Of Soil Used In The Study

Physical properties	Peat soil
Specific gravity	2.5
Natural moisture content (%)	34%
Liquid limit (%)	27%
Plastic limit (%)	41.04%
pH	3.8
Total porosity (%)	61%
Organic carbon content (%)	4.65%
Sand (%)	33 %
Silt (%)	51 %
Clay (%)	16 %

A stock solution of 10000 mg/L of phenol was prepared by dissolving analytical grade of solid phenol (Merck Chemical Limited, India) in double distilled water. The

stock solution was then diluted to various concentrations of phenol solutions (5 to 20 mg/L) for using in the batch experiment. The pH of the solution was adjusted by adding 1N HCl or 1N NaOH solutions using a pH meter (EUTECH pH 1100).

Batch Adsorption Tests

Batch adsorption tests were conducted in the laboratory to study the effect of adsorbent dosage, initial adsorbate concentrations, pH of the solutions and contact time on phenol removal efficiency by using peat soil as adsorbent. All the tests were conducted at room temperature. Various amount of adsorbent dosage (50 to 200g/L) were taken in series of 250ml capacity glass stoppered flask with 100 ml solution containing 5, 8, 10, 15 and 20 mg/L of phenol. The pH of the solution were adjusted to 7.0 ± 0.1.The glass stoppered flasks was then placed in a orbital rotary shaker and rotated at a speed of 140 rpm for 7 hours. The flasks were taken out from the shaker at predetermined time intervals (at 2, 3, 4, 5,6 and 7 hours) and solutions were filtered through 0.22µm filter paper. The residual phenol concentrations were determined spectrophotometrically after developing colour using 0.3 ml potassium ferricyanide and 0.3 ml 4-amino antipyrine solution. The residual concentration were measured using a UV/VIS spectrophotometer (Techcomp UV-2300 spectrophotometer)at a wavelength of 500µm in a 5 cm cell by standard methods [14].

The percentage of phenol removal was calculated by equation 1.

$$\text{Percentage removal of phenoll} = \left(\frac{C_0 - C_e}{C_0}\right) x100 \quad \text{.....(1)}$$

where, C_0 and C_e are the initial and equilibrium concentration of phenol in mg/L.

ANN model

ANN simulates the working principle of human brain and performs learning and prediction[15].In recent years there has been considerable interest in employing neural networks to model chemical and biochemical processes due to their ability to identify complex input-output relationship [16, 17].Atypical neural networks consist of one input layer, one or more hidden layer and one output layer. Each layer of the network consists of inter-connected processing units which are called neurons. The neurons in the hidden layers are connected to the neurons of preceding and succeeding layers by adjustable weights which enable the network to compute complex associations between inputs and outputs [18].

In the present study, the neural network toolbox of version 7 of MATLAB, Mathworks Inc. was used to develop the ANN model. A three layer feed forward neural network with tangent sigmoid transfer function (tansig) between input and hidden layer and linear transfer function (purelin) between hidden and output layer was used. The Lavenberg-Marquardt algorithm was used to train the ANN model. The inputs in the model consisted of adsorbent dosage (g/L), initial phenol concentrations (mg/L), initial solution pH and contact time(hr).The percentage removal of phenol (mg/L) was selected as output variable. The range of variables used in the model are presented in Table2.The neural network model architecture are shown in Fig.1.

Table 2: Model Variables And Their Range

Layer	Variable	Range
Input layer	Initial concentration of phenol (mg/L)	5 - 20
	Adsorbent dosage (g/L)	50 - 200
	pH	2 - 10
	Time of contact (hr)	0.5 – 7
Output layer	Phenol removal efficiency (%)	0.57-42.80

The neurons in the hidden layer were varied to optimize the model. Two hundred (200) batch experiment data were used to develop the model. The data sets were divided into training, testing and validation subsets and each of them contain 100, 50 and 50 data respectively. The input and output variables in the present study had different characteristics and importance level resulting into varied response to the neural network. The ANN model training would be more efficient if preprocessing steps are performed on the input and target data [19]. Preprocessing can be in the form of data scaling, normalization and transformation [20].

So, prior to training, the data sets were scaled in between 0 and 1 using equation 2

$$X_N = \frac{X_{act} - X_{\min}}{X_{\max} - X_{\min}} \quad \text{……..…..(2)}$$

Where X_N, X_{act}, X_{min} and X_{max} are normalized, observed, minimum and maximum values of the data series respectively. In order to compare the results of the neural network with the observed values, the rescaled output data was again post processed by converting it into denormalizing unit.

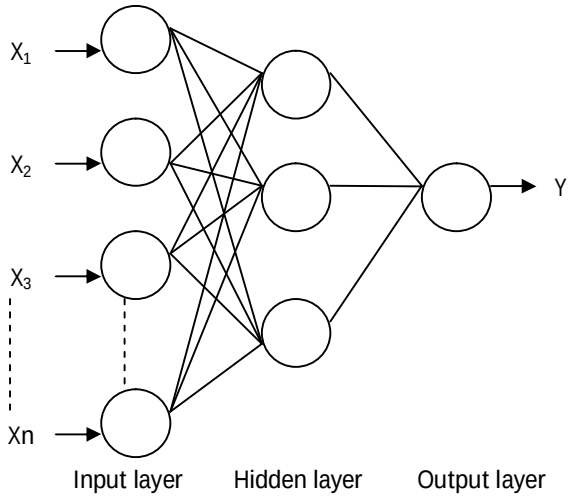

Fig.1 Neural network model architecture.

RESULT AND DISCUSSION

Batch adsorption studies

Batch adsorption studies led to standardization of the optimum condition as: initial phenol concentration (10mg/L), adsorption dose (200g/L), initial solutions pH 6 and equilibrium contact time of 6h for maximum phenol removal (42.8 %) from aqueous solution. The results were shown in Fig 2.

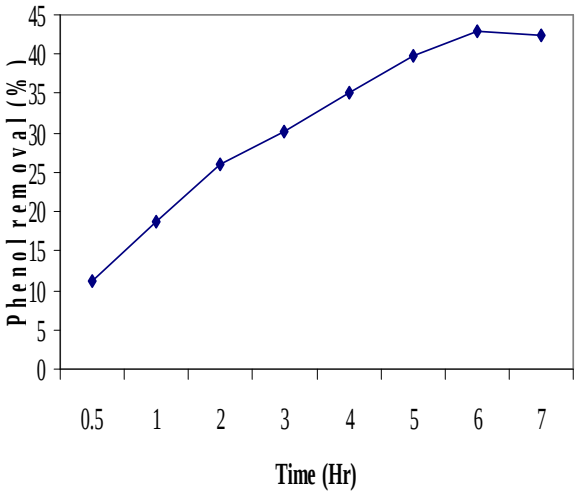

Fig. 2. Kinetics for phenol removal; Initial phenol concentration (10 mg/L); Adsorbent dose (200 g/L), Solution pH 6.

From Fig 2, it can be said that peat soil has considerable potential to be used as adsorbent for phenol removal from waste water. Studies, therefore, have been planned to predict the phenol removal efficiency from the aqueous medium by peat soil as adsorbent using ANN model.

Optimization of ANN structure

The optimum architecture of the ANN model and its parameter variation were determined based on the minimum value of the MSE of the training and prediction set [13]. The optimization was done using Lavenberg-Marquardt (LM) training algorithm. As an initial guess, two neuron was chosen in the hidden layer. With the increase of neuron numbers the MSE value was found decreasing. Fig.3. shows the relation between the MSE values and number of neuron in the hidden layer. From Fig 3 it was observed that MSE values was much higher for 2(MSE= 0.155467) and 4(MSE=0.0432374) neurons in the hidden layer. With the increase of hidden neurons from 8 to 12,the MSE value decreases from 0.0333617 to 0.0210067.With further increasing of hidden neurons the MSE value decreasing further and reached minimum value (MSE=0.00105996) at 20 hidden neurons. Hence the neural network containing 20 hidden neurons was selected as optimum case. As neuron number in the hidden layer was increased to 22, the MSE value was found slightly increased to 0.00155907. With further increase in neuron numbers in hidden layer resulted a sharp increase in the MSE value. Fig.4 illustrated the training, validation and test mean squared error for the Lavenberg-Marquardt algorithm. The training was stopped after 16 epochs.

In our present study, a three layered ANN model with tangent sigmoid transfer function (tansig) in between input layer and hidden layer and linear transfer function (purelin) in between hidden layer and output layer with Lavenberg-Marquardt training algorithm was chosen to predict phenol removal efficiency using peat soil as adsorbent.

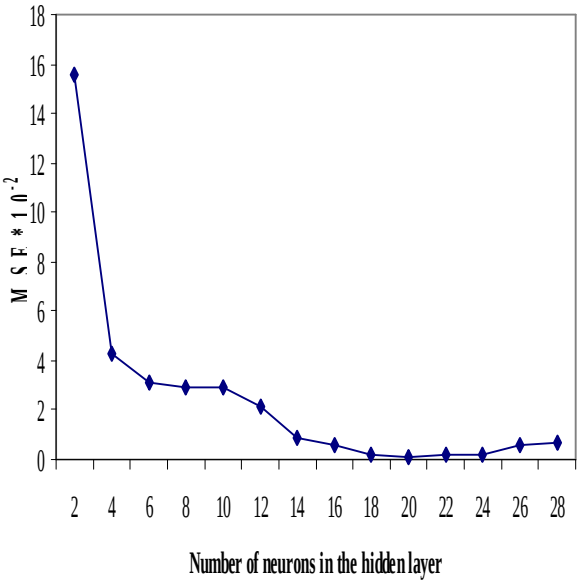

Fig.3. Relation between the MSE and number of neurons in the hidden layer

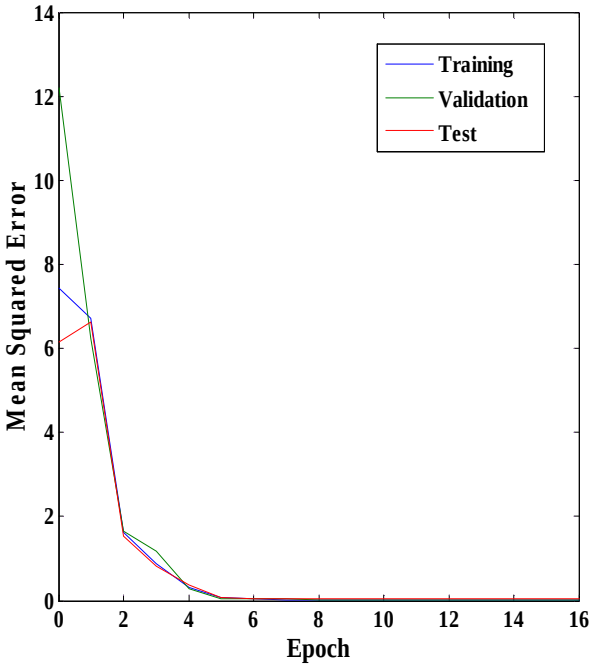

Fig.4 Training, validation and test mean squared errors for the Levenberg-Marquardt algorithm.

Fig. 5 shows the comparison between experimental phenol removal values and predicted values using the neural network model. The figure shows two lines. First one is the perfect fit A=T (predicted data equal to experimental data) on which all the data of an ideal model should lay. The other is the best fit indicated by a solid line with best linear equation A= 0.982 T +0.347.

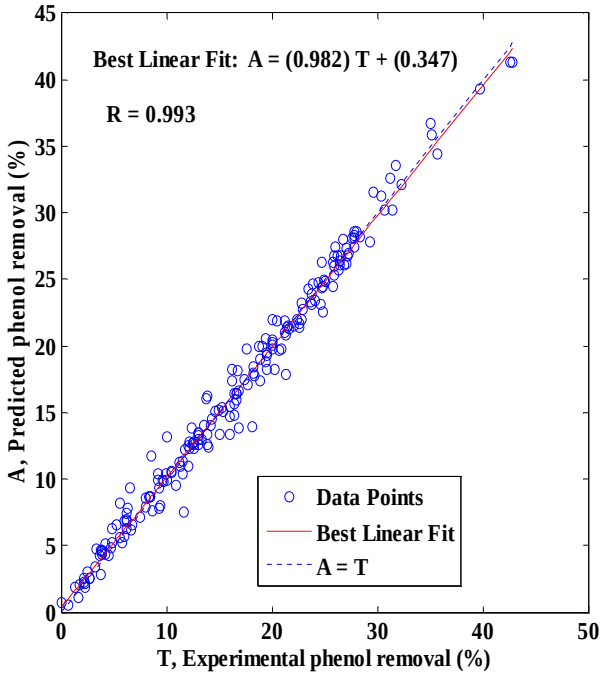

Fig.5 Comparison of experimental and ANN predicted values.

The correlation coefficient (R) of best fit line is 0.993 with MSE value of 0.00105996. The correlation coefficient closer to 1 indicates the better performance of the model. It was found that the predicted values of phenol removal efficiency by neural network model are in close agreement with laboratory batch test results.

CONCLUSION

In the present study, a three layer feed forward neural network was optimized to predict the phenol removal efficiency from aqueous solution using peat soil as adsorbent. The model consisted of Lavenberg-Marquardt back propagation training algorithm with tangent sigmoid transfer function (tansig) between input and hidden layer and linear transfer function (purelin) between hidden and output layer. The MSE value was found lowest (0.00105996) at 20 neurons in hidden layer. A regression analysis was performed between model predict value and experimental data. ANN predicted values are in close agreement with laboratory batch experimental data. The correlation coefficient (R) was found 0.993. The present studies showed that the ANN model can effectively simulate and predict phenol removal efficiency in complex adsorption process.

REFERENCES

[1]J.W.Patterson, "Wastewater treatment technology", Ann Arbor Science Inc, USA, 1975.

[2]J.Y.Yu, M.Y.Shin, J.H.Noh, and J.J. Seo, "Adsorption of phenol and chlorophenols on Ca-montmorillonite in aqueous solutions", Geoscience Journal , vol. 8, No.2 , pp.185-189, 2004.

[3]ATSDR, "Toxicological profile of phenol", U.S. Department of Health and Human Services. CAS # 108-95-2, Public Health Service, Atlanta, G.A, 1998.

[4]P.P. Mitra, and T.K. Pal,"Treatment of effluent containing phenol and catalytical conversion",Int. Chem. Eng., 41 (1),26-30, 1994.

[5]A.V. Sivanandam and T.S. Anirudhan, "Phenol removal from aqueous system by sorption on jack wood sawdust", Indian J.Chem, Technol., 2,137-142, 1995.

[6]D.K.Singh and A. Mishra,"Removal of phenolic compound from water using chemical treated saw dust", Ind. J. Env. Health, 32,345-351,1990.

[7]D.J. Bhat, D.S.Bhargava and P.S.Panesar, "Effect of pH on phenol removal in moving media reactor", Indian J. Env. Health, 25, 261-267,1983.

[8]S.N. Mukherjee, S.Kumar, A.K. Mishra and M. Fan,"Removal of phenols from water environment by activated carbon, bagasse ash and wood charcoal", Chemical Engg. Journal, 129, 133-142,2007.

[9]T.Viraraghavan, and F.Maria Alfaro,"Adsorption of phenol from wastewater by peat, fly ash and bentonite", J. Hazard. Mater.,57,59-70,1998.

[10]M.M. Mortule, J. Abdalle and A. Ghadban," Modeling phosphorus removal process using artificial neural network", BALWOIS-2010-Ohrid, Republic of Macedonia.

[11]C.Brasquet, and P.Le Cloirec,"QSAR for organics adsorption onto activated carbon in water: What about the use of neural networks?", Water Research, 33(17), 3603-3608,1999.

[12]K.V.Kumar and K.Porkodi, "Modeling the solid-liquid adsorption processes using artificial neural networks trained by pseudo second order kinetics", Chemical Engineering journal, 148(1), 20-25,2009.

[13]K. Yetilmezsoy and S. Demirel," 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, 2008.

[14]APHA, AWWA,WCF, Standard methods for examination of water and wastewater, 17th Ed., Washington, D.C,USA, 1995.

[15]B.B. Ekici and U.T. Aksoy, "Prediction of building energy consumption by using artificial neural networks", Adv. Eng. Softw. , 41(2), 141-147,2010.

[16]D.R.Baughman and Y.A.Liu, "Neural networks in bioprocessing and chemical engineering.", Academic Press, San Diego, 1995.

[17]A. Sato, Z. Sha and S.Palosaari, "Neural networks for chemical engineering unit operation.", Chem. Eng. Technol.,22,732-739,1999.

[18]K.H.Chu,"Prediction of two-metal biosorption equilibria using a neural network", The European Journal of Mineral Processing and environmental Protection, 3(1), 119-127, 2003.

[19]R.M.Aghav, S.Kumar and S.N. Mukherjee," Artificial neural network modeling in competitive adsorption of phenol and resorcinol from water environment using some carbonaceous adsorbents", Journal of Hazardous Materials, 188, 67-77,2011.

[20]T.Masters, "Practical neural network recipes in C++", Academic Press, San Diego, California,1993.