Artificial Neural Network Modeling for Adsorption of Dyes from Aqueous Solution using Rice Husk Carbon

R. D. Khonde
Assistant Professor
Department of Chemical Engineering
Priyadarshini Institute of Engineering & Technology,
Nagpur, Maharashtra State, India

S. L. Pandharipande
Associate Professor
Department of Chemical Engineering
Laxminarayan Institute of Technology, Nagpur,
Maharashtra State, India

ABSTRACT
Adsorption is one of the important industrial processes used for removal of colour, odour, turbidity & reduction of COD. In adsorption, the solute present in dilute concentration in liquid or gas phase is removed by contacting with suitable solid adsorbent so that the transfer of the component first takes place on the surface of solid and then into the pore of the solid.

The present work is aimed at exploring rice husk carbon as low cost adsorbent for removal of various dyes from synthetically prepared aqueous solutions and modeling the adsorption process using artificial neural network.

Rice husk carbon, developed in the present work at the laboratory scale, is analyzed for its BET surface area & is observed to be very effective for removal of dyes, namely bromocresol red, alizarin red, malachite green and methylene blue from their aqueous solutions. Further, the RHC developed. The present work highlighted the efficacy of ANN as an effective tool in modeling adsorption.

The ANN models developed are using elite-ANN ©.The architecture of artificial neural network is initialized & training has been carried out using the experimental data. The trained neural network is used to predict output for the given set of input parameters.

Keywords
Artificial neural networks, adsorption, modeling, dyes.

1. INTRODUCTION
The presence of dyes in effluents is a major concern due to their adverse effect to many forms of life. The discharge of dyes in the environment is worrying for both toxicological and aesthetical reasons. Industries such as textile, leather, paper, plastics, etc., are some of the sources for dye effluents. In general, dyes are poorly biodegradable or resistant to environmental conditions. Therefore it is necessary to treat the wastewaters or industrial effluents containing dyes before being discharged into the waterways. A number of chemical and physical processes such as flocculation, chemical coagulation, precipitation, ozonation and adsorption have been widely used to treat dye bearing wastewaters. However, the adsorption has been found to be superior compared to other techniques for wastewater treatment in terms of its capability for efficiently adsorbing a broad range of adsorbates and its simplicity of design. The commercially available activated carbons are still considered expensive due to the use of nonrenewable and relatively expensive raw materials such as coal, which is unjustified in pollution control applications. Therefore, in recent years, this has prompted a growing research interest in the production of activated carbons from renewable and cheaper precursors which are mainly industrial and agricultural byproducts [1,2,3,4,5].

An Artificial Neural Network (ANN) is an information processing paradigm that is inspired by the way the biological nervous system, such as brain processes information. It is composed of large number of highly interconnected processing elements (neurons) working in unison to solve specific problem [6].

The most common for chemical engineering application is Multi Layer Perception (MLP), which is a feed forward neural network. It consists of multilayer hierarchical structure, which apart from input and output layers, has at least one layer of processing units in between them. The layers between the input and output layers are termed "hidden" since they do not converse with the outside world directly. The nodes between the two successive layers are fully connected by means of weights. That is outputs from the input layer are fed to hidden layer units, which in turn, feed their outputs to the next hidden nodes. The hidden node passes the net activation through a nonlinear transformation of a linear function, such as the logistic sigmoidal or hyperbolic tangent to compute their outputs. For the training of such a MLP error back propagation algorithm suggested by Rumelhart[7] is popular. This is based on a nonlinear version of the Windro-Hoff rule known as Generalized Delta Rule (GDR). The schematic of the MLP network developed for the adsorption of dyes from aqueous solution using RHC adsorbent with two hidden layers containing five neurons each is shown in *figure 1*.

Various applications of ANN are, an approach to fault diagnosis in chemical processes[8], fault diagnosis in complex chemical plants[9], incipient fault diagnosis of chemical process[10], leak detection in liquefied gas pipeline[11,12], for estimation of mass transfer coefficient for fast fluidized bed solids[13], modeling of distillation column[14], detergent formulation[15], modeling of unsteady heat conduction in semi infinite solid[16], prediction of mass transfer coefficient in down flow jet loop reactor[17] and modeling of packed column[18] and similar other[19,20] were also reported.

2. MATERIALS AND METHODS
Rice husk is synthesized into adsorbent on laboratory scale. Rice husk was first washed with water and dried in an oven at 100^{o}C for about 6 hours. The material was then crushed in ball mill, sieved and burnt in furnace at 400^{o}C for about 10 minutes. Number of such runs had been taken.

2.1 Methodology

The present work is divided in two parts. The first part is devoted for development of rice husk carbon from an agricultural waste using thermal treatment and its analysis for measurement of surface area. The adsorption experimentation includes removal of dyes form aqueous solution, known volume of adsorbate is added to a known amount of adsorbent and once the equilibrium is reached its concentration is measured using standardized digital Colorimeter. The experimental values of % adsorption and equilibrium concentration are calculated for each adsorbate with variable amount of adsorbent as given in *Table 1*.

The second part is devoted for development of artificial neural network model for estimation of equilibrium concentration of different adsorbates and their % adsorption.

2.2 Developing ANN model

The procedure of designing an ANN model is as follows:

- Specifying the number of inputs and outputs for the network
- Creating a database of specified input-output variables
- Selection of network type, number of layer, number of neurons and activation function of each layer
- Training of the network
- Checking the performance and precision of the trained neural network; changing and retraining of network as per accuracy level
- Validation on a set of test data

In present work, ANN model developed is using elite-ANN © [21], a back propagation network with three inputs (adsorbate coding, initial concentration of adsorbate and adsorbent dosing), two hidden layers with five neurons each and two outputs (equilibrium concentration and % adsorption) for prediction of concentration of adsorbate in a wide range of wavelength and optical density, shown in *figure 1*.

The topology of ANN architecture is as given in *table 2*. *Table 3* shows actual and predicted values of equilibrium concentration and % adsorption for training data set, whereas *table 4* shows actual and predicted values of equilibrium concentration and % adsorption for the test data set. For ANN modeling, each adsorbate is coded with number like 30 for bromocresol red, 60 for alizarin red, 80 for malachite green and 90 for methylene blue. The performance of ANN model is evaluated by the relative error and mean squared error (MSE).

Table 1: Total Data for ANN Modeling

Adsorbate	Initial concentration, C_o (mg/lit)	Amount of adsorbent, W (gm)	Amount of adsorbate adsorbed per unit amount of adsorbent, q_e (mg/gm)	% removal of adsorbate
Bromocresol Red	1000	2	39	78
	1000	4	21.5	86
	1000	6	14.91667	89.5
	1000	8	11.5625	92.5
	1000	10	9.375	93.75
Alizarin Red	100	2	3.85	77
	100	4	2.188	87.5
	100	6	1.576	94.58
	100	8	1.224	97.92
	100	10	0.988	98.75
Malachite Green	500	0.5	98.75	98.75
	500	1	49.583	99.17
	500	1.5	33.056	99.17
	500	2	24.844	99.38
	500	2.5	19.875	99.38
	500	3	16.597	99.58
	500	4	12.448	99.58
Methylene Blue	500	1	48.464	96.93
	500	1.5	33.021	99.06
	500	2	24.974	99.9
	500	2.5	19.99	99.95
	500	3	16.667	100

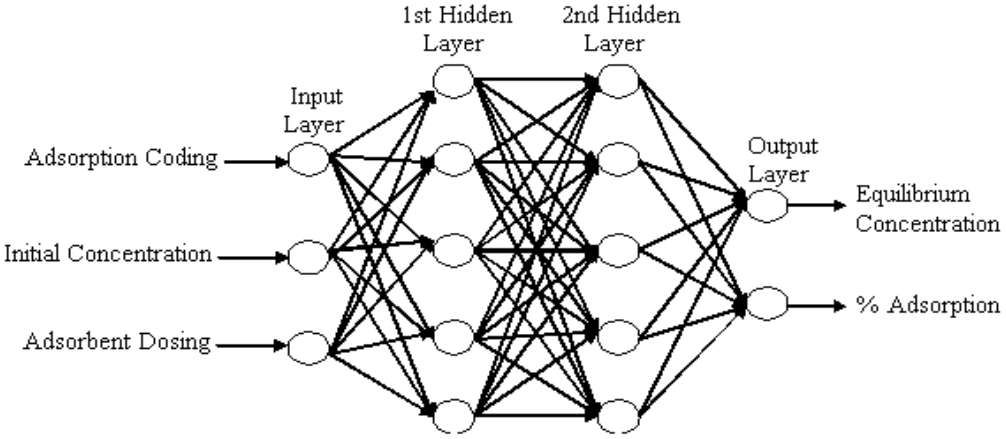

Figure 1: Artificial Neural Network Architecture

Table 2: Neural network topology for ANN model using elite-ANN

Number of Neurons				**Data Points**		**Learning rate**
Input parameters	2nd hidden layer	3rd hidden layer	Output parameters	Training	Test	
3	05	05	2	18	4	0.3
Iteration termination = 212380 Time in milliseconds = 26473		First momentum factor = 0.75 Second momentum factor = 0.01		RMSE for training data = 0.025 RMSE for test data = 0.024		
Input Parameters: Adsorption Coding, Initial Concentration, Adsorbent Dosing				Output Parameters: Equilibrium Concentration, % Adsorption		

Table 3: Actual and predicted values for training data set

1th Input	**2th Input**	**3th Input**	**1th Actual output**	**1th Predicted output**	**2th Actual output**	**2th Predicted output**
Adsorbate coding	**Initial concentration, C_o (mg/lit)**	**Amount of adsorbent, W (gm)**	**Equilibrium adsorption of adsorbate per unit amount of adsorbent, q_e (mg/gm)**		**% adsorption**	
30	1000	2	39	39.8108	78	77.53448
30	1000	4	21.5	20.9445	86	87.845
30	1000	6	14.91667	13.8035	89.5	88.67972
30	1000	10	9.375	8.67525	93.75	93.05009
60	100	2	3.85	3.35197	77	76.97116
60	100	4	2.188	2.44731	87.5	88.44251
60	100	6	1.576	1.29069	94.58	95.99177
60	100	10	0.988	0.8081	98.75	98.13324
80	500	0.5	98.75	90.6463	98.75	97.93034
80	500	1	49.583	53.5985	99.17	99.67745
80	500	1.5	33.056	31.0649	99.17	99.86529
80	500	2	24.844	23.2317	99.38	99.91076
80	500	3	16.597	17.5797	99.58	99.93993
80	500	4	12.448	15.1463	99.58	99.95159
90	500	1	48.464	48.5422	96.93	99.76813
90	500	2	24.974	22.3709	99.9	99.92453
90	500	2.5	19.99	19.4598	99.95	99.93798
90	500	3	16.667	17.802	100	99.94555

Table 4: Actual and predicted values for test data set

1th Input	2th Input	3th Input	1th Actual output	1th Predicted output	2th Actual output	2th Predicted output
Adsorbate Coding	Initial concentration, C_o (mg/lit)	Amount of adsorbent, W (gm)	Equilibrium adsorption of adsorbate per unit amount of adsorbent, q_e (mg/gm)		% adsorption	
30	1000	8	11.5625	10.55648	92.5	90.38971
60	100	8	1.224	1.35749	97.92	97.90939
80	500	2.5	19.875	19.64398	99.38	99.9296
90	500	1.5	33.021	28.87818	99.06	99.89282

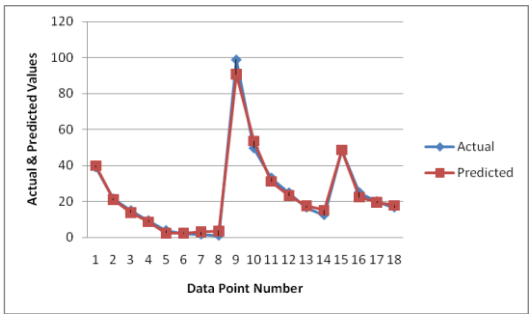

Figure 2: Comparison of actual and predicted values of equilibrium concentration of adsorbates for training data set

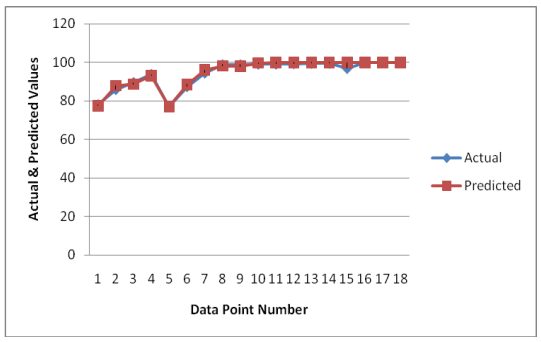

Figure 3: Comparison of actual and predicted values of % adsorption of adsorbates for training data set

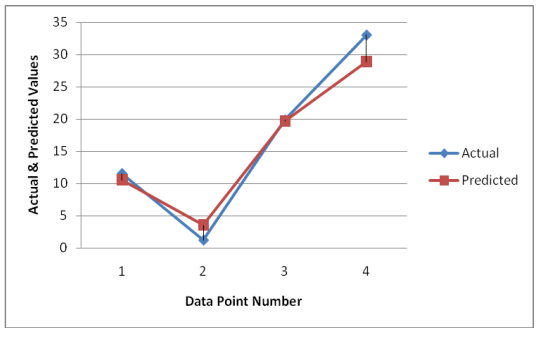

Figure 4: Comparison of actual and predicted values of equilibrium concentration of adsorbates for test data set

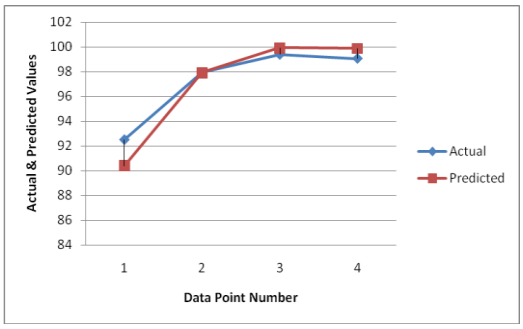

Figure 5: Comparison of actual and predicted values of % adsorption of adsorbates for test data set

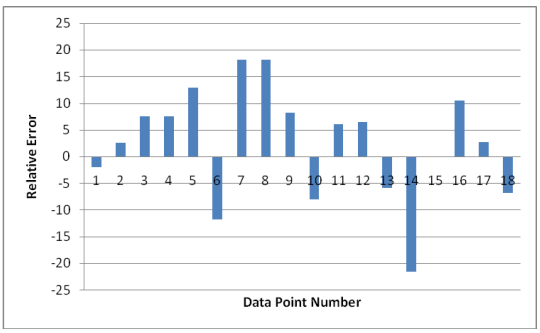

Figure 6: % Relative error for equilibrium concentraiton of adsorbates for training data set

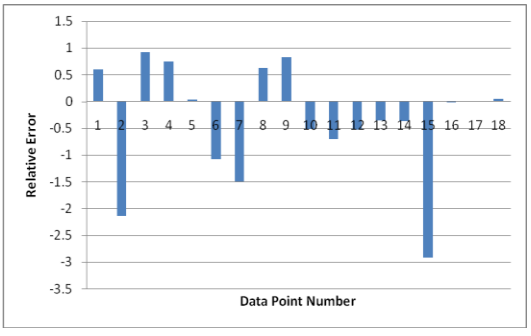

Figure 7: % Relative error for % adsorption of adsorbates for training data set

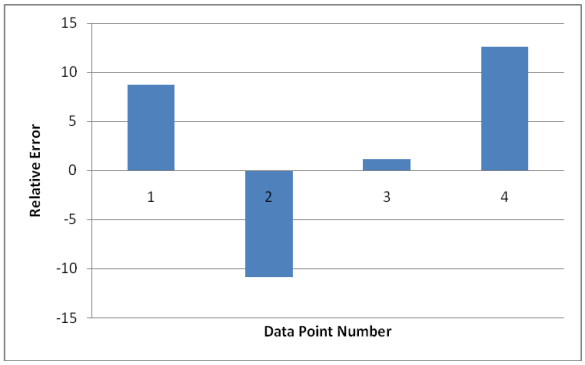

Figure 8: % Relative error for equilibrium concentraiton of adsorbates for test data set

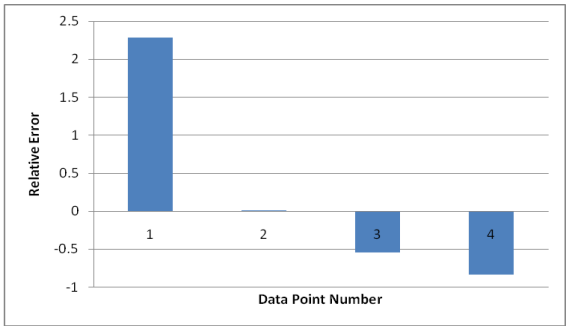

Figure 9: % Relative error for % adsorption of adsorbates for test data set

3. RESULTS & DISCUSSION

The yield of rice husk carbon (RHC) synthesized in present work is 50 % having surface area of 208.637±3.4941 m^2/gm as determined by BET analyzer.

The comparison of actual and predicted values of equilibrium concentration and % adsorption of various adsorbates like bromocresol red, alizarin red, malachite green and methylene blue have been plotted as shown in *figure 2* and *figure 3* for training data set; and *figure 4* and *figure 5* for test data set. As can be seen from these graphs, actual and predicted values are very close to each other. However for substantiating the claim of accuracy of prediction further, relative error have been calculated plotted as shown in *figure 6* and *figure 7* for training data set and *figure 8* and *figure 9* for test data set.

4. CONCLUSION

It can be concluded that the ANN model developed has excellent accuracy and the model can be effectively used for prediction of % adsorption and equilibrium concentration of dyes on rice husk carbon adsorbent. The unique feature of the ANN model developed is that it gives substitute for conventional adsorption isotherm that enables the user to incorporate the multiple adsorbates in the same correlation with ease & high accuracy. The work is demonstrative & can be extended for more combinations of adsorbate & adsorbent in a single ANN model.

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