Comparative Study of Topology of ANN Models for Adsorption of Colouring Agents from Aqueous Solutions using Adsorbents Synthesized from Agricultural Waste Material

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ABSTRACT
The ability of some solids to remove colour from solutions containing dyes has been known for over a century. Activated carbon has been quite successful for removal of impurities from exhaust gas and waste water streams. The highly porous nature of the carbon provides a large surface area for contaminants to get deposited. Artificial neural network is a black box modeling tool & is applied for several chemical engineering operations. In the present work ANN models 1,2 & 3 having different topologies have been developed for correlating input parameters like name of adsorbate, name of adsorbent, initial concentration of solute in aqueous solution & quantity of adsorbent with output parameters such as % adsorption & equilibrium concentration of solute in adsorbent. The novel feature of present work is selection of suitable ANN model based on topology.

Keywords
Artificial Neural Network, modeling, topology, adsorption

1. INTRODUCTION
The ability of some solids to remove colour from solutions containing dyes has been known for ages. Similarly, air contaminated with unpleasant odours could be rendered odourless by passage of the air though a vessel containing charcoal. Indeed, the adsorption is continually advancing as new and improved as the applications occur in competition with other well-established process technologies, such as distillation and absorption. Attempts at understanding how solutions containing dyes could be bleached, or how obnoxious smells could be removed from air streams, led to quantitative measurements of the concentration of adsorbable components in gases and liquids before and after treatment with the solid used for such purposes. The classical experiments of several scientists including Brunauer, Emmett and Teller, McBain and Bakr, Langmuir, and later by Barrer, all in the early part of the twentieth century, shed light on the manner in which solids removed contaminants from gases and liquids.

Activated carbon has been quite successful for removal of impurities from exhaust gas and waste water streams. The highly porous nature of the carbon provides a large surface area for contaminants to get deposited. The adsorption takes place because of the attractive force between the molecules. There is wide variety of activated carbons which exhibit different characteristics depending upon the raw materials and the activation techniques used in their synthesis. Agricultural waste materials like straw, leaves, stem, seeds and husk can effectively be converted in to activated carbon. [1], [2],[3],[4]. The objective of the present work is to utilize waste materials like Rice Husk, Saw Dust & Sugarcane Baggasse by converting them into adsorbent for various applications followed by modeling the adsorption process using artificial neural network. It also encompasses the comparative topology study in arriving at optimal ANN model.

An Artificial Neural Network (ANN) is an information processing interdisciplinary theme based on the working principle of the biological nervous system, similar to the way brain processes information. It is composed of large number of highly interconnected processing elements called neurons or nodes working in a network to solve specific problem[5],[6]

The most common type of artificial neural network for chemical engineering application is Multi Layer Perception, which is a feed forward neural network. It consists of multilayer hierarchical structure, which has at least one layer of processing units in between input and output layers. The layers between the input and output layers are termed "hidden" since they do not communicate with the outside world directly. The nodes between the two successive layers are fully connected by means of constants called as weights. The outputs of the input layer nodes are fed to hidden layer nodes, which in turn, feed their outputs to the next hidden nodes. The hidden node passes the net activation through a nonlinear transformation, 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. The schematic of the typical architecture of the network used in developing models is shown in fig 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],[21],[22] were also reported.

Table no1: Artificial Neural Network topologies for models 1, 2 & 3

Name of Model	Number of Neurons					Learning rate	RMSE	
	Input Parameters	Output Parameters	1st hidden layer	2nd hidden layer	3rd hidden layer		Training data set 27 points	Test data set 9 points
ANN Model 1	04	02	00	05	05	0.3	0.02436	0.05034
ANN Model 2	04	02	10	10	10	0.6	0.28116	0.02306
ANN Model 3	04	02	00	10	10	0.5	0.01902	0.05798

2. MATERIALS AND METHODS

The special feature of ANN model is that it can incorporate parameters which are otherwise difficult to be quantified such as type of adsorbent or adsorbate. In the present work effort has been made to develop a correlation involving multiple adsorbates & multiple adsorbents in a same model.

Adsorption experiments have been carried out. Adsorbents synthesized from agricultural waste materials like sugarcane baggasse, saw dust and rice husk are used for removal of colour agents lie potassium dichromate, methyl violet and methylene blue[23] .

ANN models 1, 2 & 3 having different topologies have been developed. Input parameters like coded numbers for adsorbates & adsorbents, initial concentration of solute in aqueous solution & quantity of adsorbent are correlated with output parameters like % adsorption & equilibrium concentration of solute in adsorbent. The table no 1 gives the neural network topology used for developing ANN models 1, 2 &3. The total data set is divided into two parts. One part is of the total dataset is called as training data set whereas the other part is called as test data set. The training of the ANN is done by using the training data set and its effectiveness in estimation is judged by the test data set. The software used in present work is elite-ANN [24].

3. RESULTS & DISCUSSIONS

ANN models 1, 2 & 3 developed are used for prediction of the output parameters % adsorption and equilibrium concentration for all the data points of training and test data sets. Comparison of the actual and predicted output values has been carried out. Graphs are plotted between actual and predicted values using ANN models1, 2&3 of % adsorption and equilibrium concentration for training data set as shown in fig 2 & 3 respectively. There is a close agreement between actual and predicted values.

Similarly fig no 4 & 5 show the comparison between actual and predicted values using ANN model 1,2&3 for output parameters % adsorption and equilibrium concentration for test data set respectively. The final selection of suitability of the ANN model is taken based on the comparison of relative error values of both the output parameters for all the data points using ANN models 1, 2 & 3. Fig no 6 & 7 and fig no 8 & 9 show the comparison of these values of relative error for % adsorption and equilibrium concentration for training and test data set respectively. It can be inferred that the ANN model 1 is most suitable for estimation of % adsorption and equilibrium concentration. The topology of ANN model is simple as compared to ANN models 2 and 3. The present work has highlighted that increase in the number of hidden layers and number of neurons in each layer does not necessarily lead to a model with high accuracy of predictions.

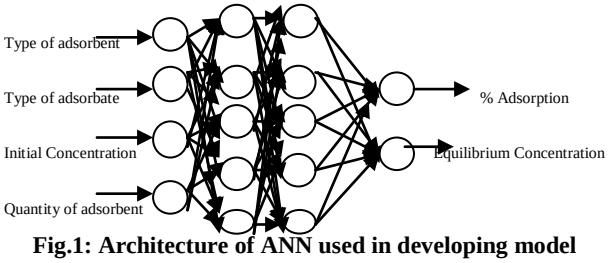


Fig.1: Architecture of ANN used in developing model

4. CONCLUSION

The novel feature of present work is the utilization of ANN modeling tool for estimation of % of adsorption & final equilibrium concentration as a function of type of adsorbate, type of adsorbent & quantity of adsorbent. The utility of model is in its validation and given the relative error for the test data set which is in the range of 0.1 to 8 %, the model is acceptable. The parameter which could not be quantified and thus cannot be included in conventional mathematical model namely type of adsorbate, type of adsorbent has been successfully incorporated in present ANN model. It can be concluded that the present work is successful in developing a suitable ANN model. The other notable feature of present work is developing ANN models for different topology. The number of hidden layers and number of neurons in each hidden layer is varied. Three different topologies involving two and three hidden layers and number of neurons from five to ten have been tried. Based on the accuracy levels of prediction using ANN models 1, 2 and 3 using different topologies it can be concluded that the model based on two

hidden layers and five numbers of neurons each has better accuracy for training and test data set.

Figure 2: Comparison of actual & predicted values of % Adsorption using ANN models 1, 2 &3 for training data set

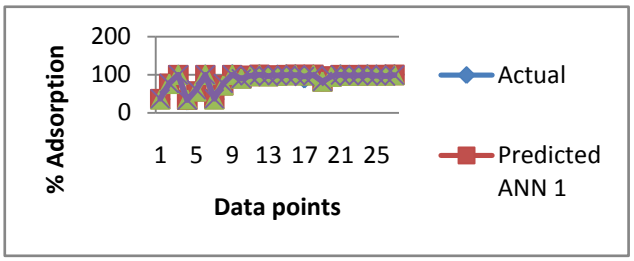


Figure 3: Comparison of actual & predicted values of equilibrium concentration using ANN models 1,2 &3 training data set

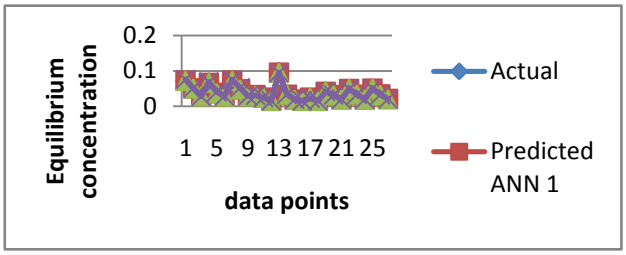


Figure 4: Comparison of actual & predicted values of equilibrium concentration using ANN models 1,2 & 3 of % Adsorption for Test data set

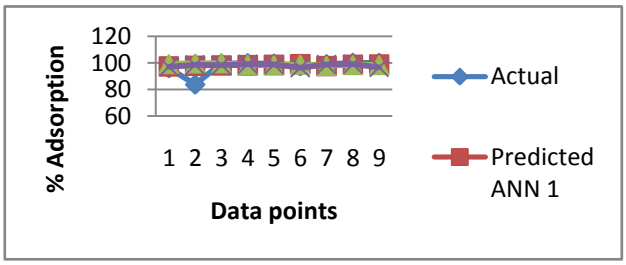


Figure 5: Comparison of actual & predicted values of equilibrium concentration using ANN models 1, 2 & 3 for test data set

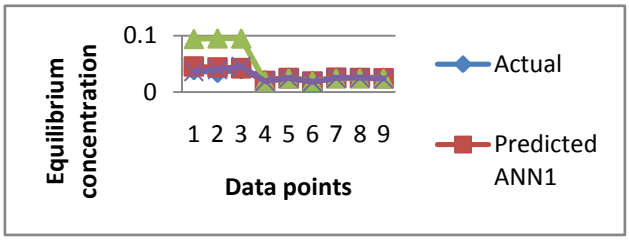


Figure 6: Comparison of relative error of % adsorption of ANN models 1, 2 & 3 for training data set

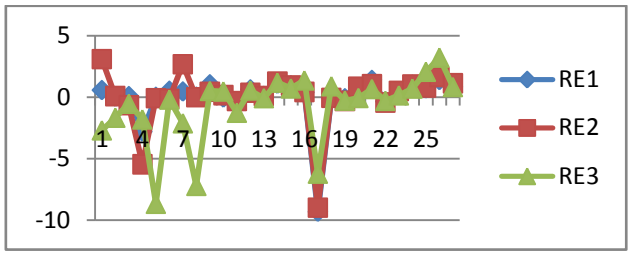


Figure 7: Comparison of relative error of equilibrium concentration of ANN models 1, 2 & 3 for training data set

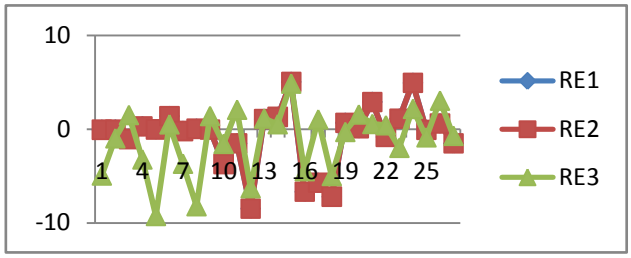


Figure 8: Comparison of relative error of % adsorption of ANN models 1,2 & 3 for test data set

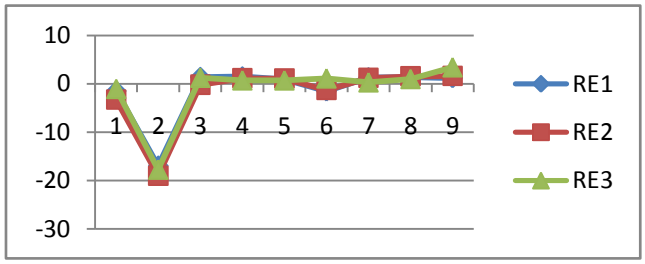
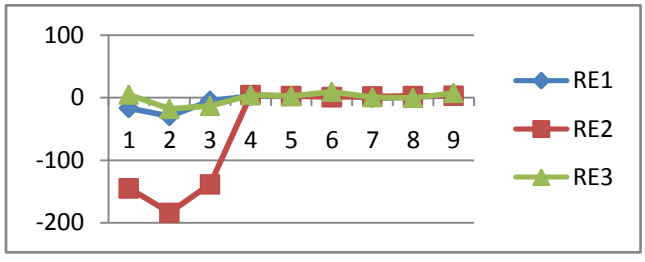


Figure 9: Comparison of relative error of equilibrium concentration of ANN models 1, 2 & 3 for test data set



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