International Journal of Engineering Sciences & Emerging Technologies, Feb. 2013.
ISSN: 2231 – 6604 Volume 4, Issue 2, pp: 27-36 ©IJESET

ARTIFICIAL NEURAL NETWORK APPROACH FOR MODELING OF NI(II) ADSORPTION FROM AQUEOUS SOLUTION USING AEGEL MARMELOS FRUIT SHELL ADSORBENT

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ABSTRACT

The rapid increase in population and growth of industrialization worldwide has resulted in deterioration in quality of water. Industrial processes have introduced substantial amounts of potentially toxic heavy metals into the environment. Which are non-biodegradable and harmful to the human health. Adsorption is found to be promising technique for removal of heavy metal ions from aqueous solution. Due to the complexity and nonlinearity of the behavior of the adsorption processes, the conventional mathematical models correlating the governing adsorption parameters In present work Artificial neural networks have been applied for modeling applications related to adsorption studies. The adsorption of Ni (II) ions from aqueous solution is 81-88% depending upon process condition. Two ANN models S-1 & S-2 are developed for the estimation of concentration of Ni (II) ions from aqueous solution based on the correlation between the optical densities of the solutions as determined by the digital colorimeter with the Ni (II) ion concentration present in the solution. Three ANN models NS, NM & NC are developed for adsorption studies. The present work could highlight the novel feature of the ANN model in estimation of concentration of Ni (II) ions present in aqueous solution. It is indicative & representative of several possible applications of artificial neural network modeling in the area of adsorption involving several possible combinations of adsorbents & adsorbents.

KEYWORDS: *Artificial Neural Network, modeling, Ni (II) ions, adsorption, aegel marmelos fruit shell adsorbent.*

I. INTRODUCTION

The rapid increase in population and growth of industrialization worldwide has deteriorated the quality of water. It is deteriorating day by day. Industrial processes have introduced substantial amounts of potentially toxic heavy metals into the environment. These heavy metals are non-biodegradable and harmful to the human health. The removal of heavy metals from the waste water is necessary before it is discharged into the main water bodies. There are several methods suggested literature which includes ion exchange, co-precipitation, membrane technology, filtration & adsorption. Adsorption is one of the promising techniques due to its low cost & ease of operation. The effectiveness of removal of metallic ions using adsorption is dependent upon the process conditions such as temperature, quantity of the feed mixture, concentration of adsorbate in feed and the type & quantity of adsorbent used. Development of different types of adsorbents with appropriate pore size distribution, large surface area, low cost & biodegradability is need of the hour because of the situations involving different types of adsorbates to be removed. Several efforts are being made in synthesizing adsorbents from agricultural waste materials. The basis of separation of adsorbate from the feed mixture onto the solid adsorbent is governed by the difference between the concentrations of the adsorbate in liquid & solid phases as compared to their equilibrium concentrations. Mathematical models have been employed in correlating these equilibrium conditions. Because of the complexity of adsorption process very often these models fail to predict.

II. ARTIFICIAL NEURAL NETWORK

Artificial Neural Network (ANN) is becoming a possible alternative modeling tool for various processes & operations involving nonlinear multivariable relationships. ANN is also called as black box modeling tool with its working principle based on the functioning of the biological neural network. It consists of highly interconnected processing elements called as neurons or nodes acting in perfect unison to solve a specific problem.

There are several types of ANN architecture, however Multilayer Perceptron (MLP) is observed to be most common for chemical processes. It is basically a feed forward neural network. It has a multilayer structure consisting of one input & output layer and at least one hidden layer in between them. The number of nodes in input and output layers is decided by the number of independent and dependent parameters defining the process whereas the selection of number of hidden layers is dependent on the complexity of the process. The nodes in successive layers are interconnected with each other through connectionist constants called as weights. The data is transferred in the form of array of matrix from input layer to output layer through hidden layers. The output signal is compared with the target value to generate error signal. Training of the network is to be carried out to minimize the error by adjusting the weights using appropriated algorithm [1,2,3].

ANNs are used to model input and output data. There are number of interdisciplinary applications of ANN reported in robotics, medical sciences, metallurgy, accounting, engineering etc. The chemical engineering applications of ANN include hydrodynamics of packed column [4], leak detection in pipelines[5], prediction of mass transfer coefficient in downflow jet loop reactor using[6], modeling combined VLE of four quaternary mixtures[7], unsteady state heat conduction in semi infinite solids[8] & fault diagnosis[9].

ANN is also effectively being used in modeling various aspect of adsorption studies that include estimation of concentration of heavy metals from aqueous solution[10], standardization of digital colorimeter[11], modeling Zn(II) adsorption from Leachate using a new biosorbent[12], adsorption of dyes from aqueous solution using rice husk carbon[13], adsorption of textile dye on organoclay[14], metal ions sorption on chitosan foamed structure-Equilibrium & dynamics of packed column for adsorption[15] etc.

The present work aims at developing two Artificial Neural Network models related to process involving adsorption studies. The first ANN model addresses to the standardization of colorimeter for correlating the concentration of Ni(II) ions present in aqueous with optical density. The other ANN model is devoted for adsorption equilibrium, correlating the initial concentration of Ni(II) ion in the feed mixture & the adsorbent dosage as input parameters with the three output parameters such as, equilibrium concentrations of Ni(II) ion on solid & liquid phases and the percent adsorption achieved.

The paper is presented in the sections that include the methodology adopted in generation of the experimental data for developing the two models followed by the details of the topology of the ANN models used. The results and discussion has been done based upon the comparison of the actual and the predicted values for the two best suited ANN models developed. The paper concludes highlighting the utility and effectiveness of the ANN in adsorption studies.

III. MATERIAL AND METHODS

3.1 Material for adsorbent

The adsorbent that is synthesized from aegel marmelos fruit shell by thermal method has been employed in the adsorption studies of the present work[16].

3.2 Methodology

The present work is divided into two parts. The first part of the present work is related to the estimation of optical density of samples of aqueous solution having known concentration of Ni(II) present. The ANN model is developed correlating the concentration of Ni(II) ions in aqueous solution with optical density of the aqueous solution determined using digital colorimeter. The second part of

the present work is related to the adsorption experimentation that includes removal of Ni(II) from aqueous solution using adsorbent synthesized from aegel marmelos fruit shell. For this known volume of Ni(II) ions solution is added to a known amount of adsorbent and once the equilibrium is reached, the optical density of the final mixture is determined after filtration. The concentration of Ni(II) ion in final solution is obtained by using the ANN model developed in part I. The experimental values of equilibrium concentration (mg/ml), amount of adsorbate adsorbed per unit amount of adsorbent (mg/gm) and % adsorption are calculated for the various dosage of adsorbent. Artificial neural network models are developed for correlating the initial concentration of Ni(II) ion in feed, adsorbent dosage with the equilibrium concentration of Ni(II) ions on solid & liquid phases and the percent adsorption achieved.
In this study, elite-ANN© is used in developing the all ANN models [17].

IV. RESULT AND DISCUSSION

4.1 Part I: Developing ANN model for standardization of Digital colorimeter

The objective of this part of the present work is developing ANN models correlating the concentration of Ni(II) in aqueous solution with its optical density as determined by using digital colorimeter. This may be referred as ANN model for standardization of digital colorimeter for estimation of Ni(II) ions in aqueous solution.

There is one input parameter as optical density and one output parameter as concentration of Ni(II) ions (gm/ml).

Two different ANN models S-1 & S-2 are developed for two different stock solution sets having ten data points each. The neural network architecture is as shown in Figure 1.

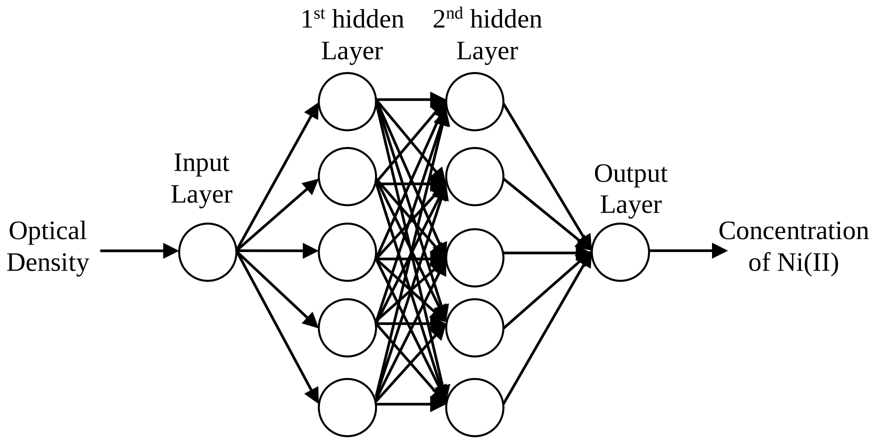

Figure 1. Neural Network Architecture for ANN model S-1 & S-2

The details of the topology of ANN models developed for standardization of digital colorimeter is given in Table 1. Both the models S-1 & S-2 developed have good accuracy levels in the range of 1-10% root mean square error (RMSE).

Table 1. Neural Network Topology for standardization of colorimeter

Model	Number of Neurons					RMSE
	Input layer	1st hidden layer	2nd hidden layer	3rd hidden layer	Output layer	Training data set
S-1	1	00	05	05	1	0.1094
S-2	1	00	05	05	1	0.0105
Number of Iterations = 50000						
Input parameter: Optical density of aqueous solution Output parameter: Concentration of Ni (II) ions in aqueous solution						

The accuracy of prediction of ANN models S-1 & S-2 is evaluated by comparing the actual and the predicted values.

Figures 2 and 3 depict the comparison of actual and predicted values for concentration of Ni(II) ions for ANN models S-1 & S-2 respectively developed for standardization of colorimeter.

As can be seen from these graphs the accuracy of the prediction is fairly good and acceptable.

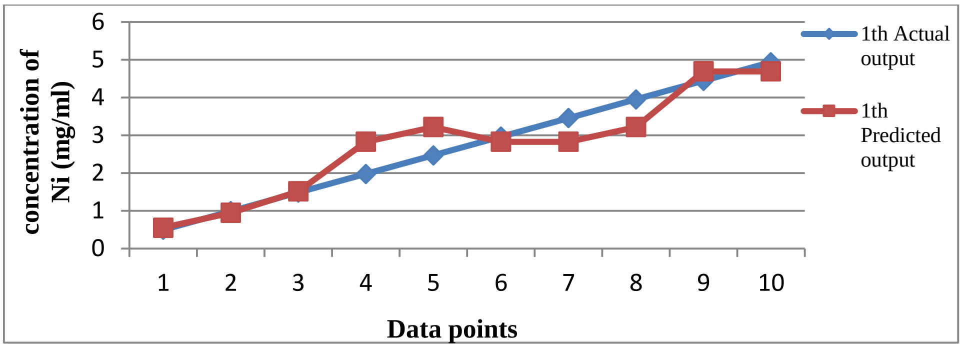

Figure 2. Comparison of actual and predicted values of concentration of Ni(II) for model S-1

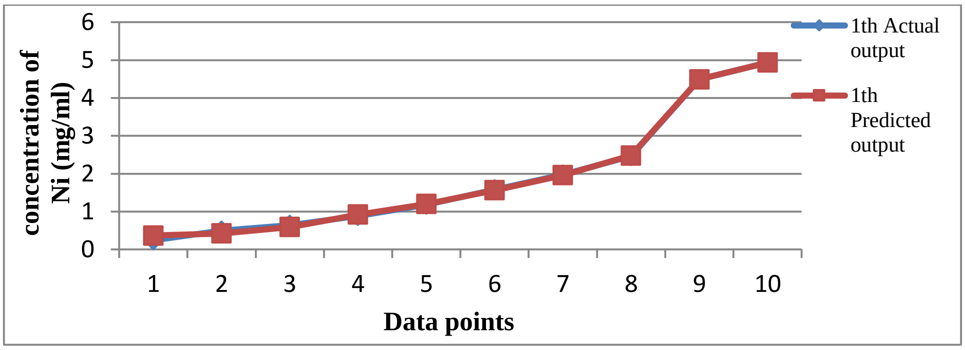

Figure 3. Comparison of actual and predicted values of concentration of Ni(II) for model S-2

The concentration of Ni(II) ions in final solution C_e as obtained after adsorption is estimated by using ANN models S-1 & S-2 developed in part 1. The models S-1& S-2 are employed in estimation of concentrations of Ni(II) ions remained in the final solutions after the adsorption as tabulated in Table 2.

The % adsorption of Ni(II) is estimated using the following formula:

% adsorption= $(C_o - C_e)/C_o \times 100$

Where, C_o is the initial concentration of Ni(II) (mg/ml), C_e is the equilibrium concentration of Ni(II) ions (mg/ml)

The calculated values of equilibrium concentration of Ni(II) ions in solid & liquid phases and % adsorption obtained is as given in the Table 2.

The adsorption of Ni(II) ions from aqueous solution is 80-88% depending on the process condition.

Table 2. Total data for ANN modeling of adsorption studies

Initial concentration C_o (mg/ml)	Amount of adsorbent (gm)	Equilibrium concentration C_e (mg/ml)	Amount of adsorbate adsorbed per unit amount of adsorbent (mg/gm)	Percentage adsorption
4.938	1	0.607	216.5	87.7
4.938	3	0.943	66.58	80.9
4.938	5	0.569	43.69	88.47
2.324	1	0.421	95.11	81.86
2.324	3	0.369	32.57	84.09

2.324	5	0.31	20.14	86.66
Input parameters: Initial concentration, Amount of adsorbent Output parameters: Equilibrium concentration, Amount of adsorbate adsorbed per unit amount of adsorbent, Percentage adsorption.				

4.2 Part II: Developing ANN models for adsorption studies

The objective of this part of the work is to correlate two input parameters initial concentration of Ni(II) in aqueous solution and adsorbent dosage with three output parameters that include equilibrium concentration of Ni(II) ions in aqueous solution, amount of adsorbate adsorbed per unit amount of adsorbent and % adsorption by developing ANN models. The data set as given in table 2 is used for this purpose.

Three ANN models NS, NM & NC having different topology as given in table 3 are developed.

Figure 4 shows a typical architecture of one of the models NS developed.

The snapshot of elite-ANN© in run mode & the variation of error versus iteration during training mode for developing "NM model" are shown in Figures 5 and 6 respectively.

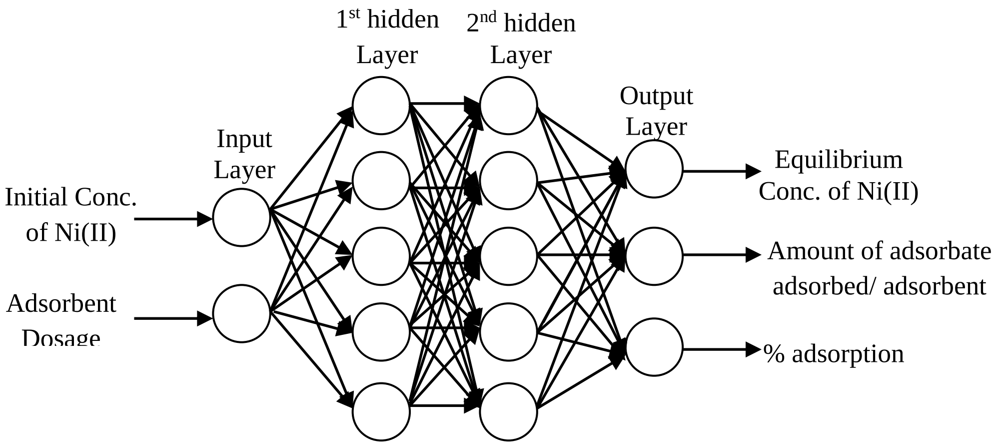

Figure 4. Neural Network Architecture for ANN model NS

Table 3. Neural network topology

Model code	Number of Neurons					RMSE
	Input layer	1st hidden layer	2nd hidden layer	3rd hidden layer	Output layer	Training data set
NS	2	00	05	05	3	0.0024
NM	2	00	10	10	3	0.0014
NC	2	10	10	10	3	0.0596
Number of Iterations = 50000						
Input parameters: Initial concentration Ni(II) ions, adsorbent dosage Output parameters: Equilibrium concentration of Ni (II) ions, amount of adsorbate adsorbed per unit amount of adsorbent, % adsorption						

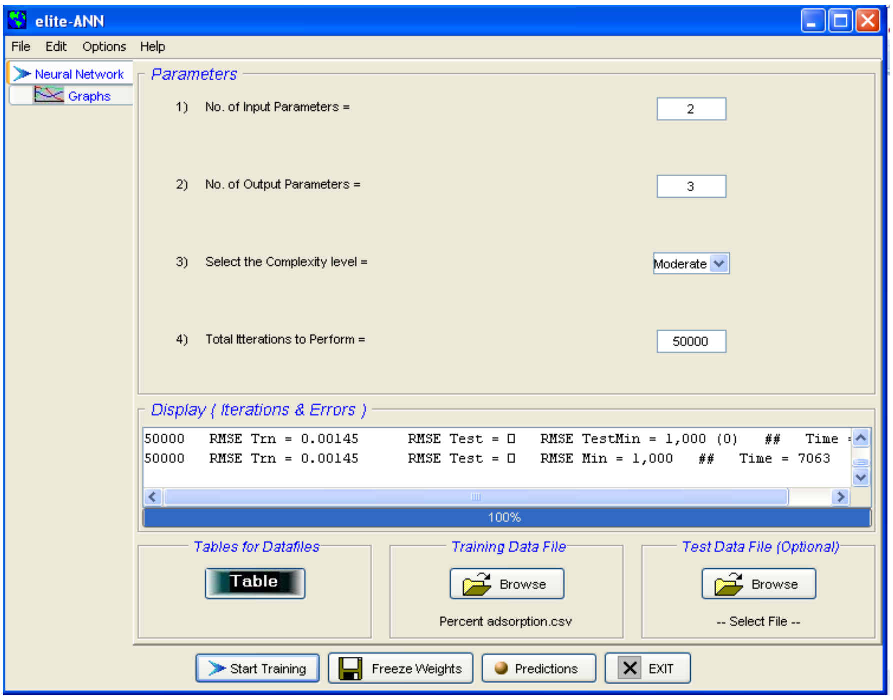

Figure 5. Snapshot of elite-ANN in run mode

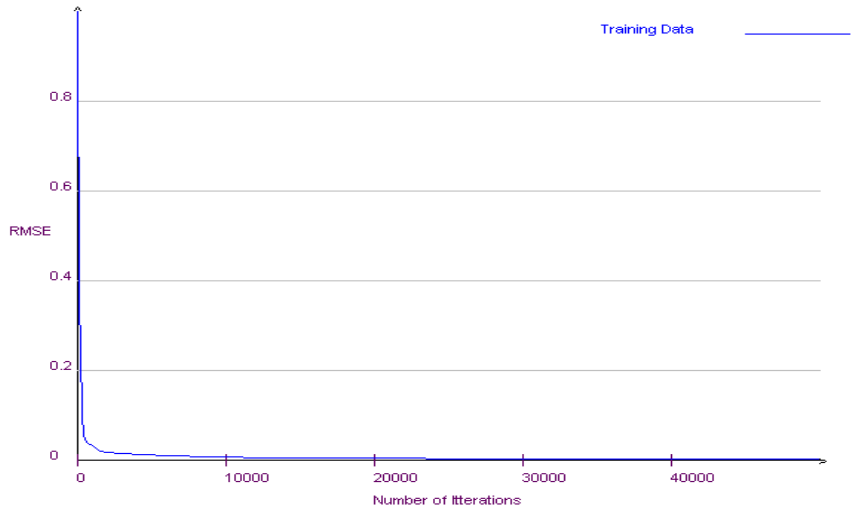

Figure 6. Iterations and corresponding RMSE for training set during developing NM model

The effectiveness of ANN model is dependent on its accuracy of prediction. Figures 7, 8 & 9 show the graphs plotted between actual & predicted values obtained using ANN models NS, NM and NC for the output parameters; equilibrium concentration of Ni(II), amount of adsorbate adsorbed per unit amount of adsorbent and % adsorption respectively.

Based on the RMSE for training data set as given in Table 3, ANN model NM is found to be highly accurate. The claim of accuracy of NM model is further validated by calculating % relative error for all the data set of output parameters. Table 4 shows the range of % relative error.

% relative error = (actual value – predicted value)/actual value × 100

Figures 10, 11 & 12 show the % relative error for the equilibrium concentration of Ni(II) ions, amount of adsorbate adsorbed per unit amount of adsorbent and %adsorption for the respective data points respectively.

Table 4. Distribution of % relative error for output parameters using ANN model NM

Output Parameters	**% relative error Training data set = 06 points**			
	≤ ±0.001	±0.001- 0.005	±0.005 - 0.01	≥ ±0.01
Equilibrium concentration of Ni(II) ions	1	0	2	3
Amount of adsorbate adsorbed per unit amount of adsorbent (mg/gm)	0	1	1	4
% adsorption	4	0	0	2

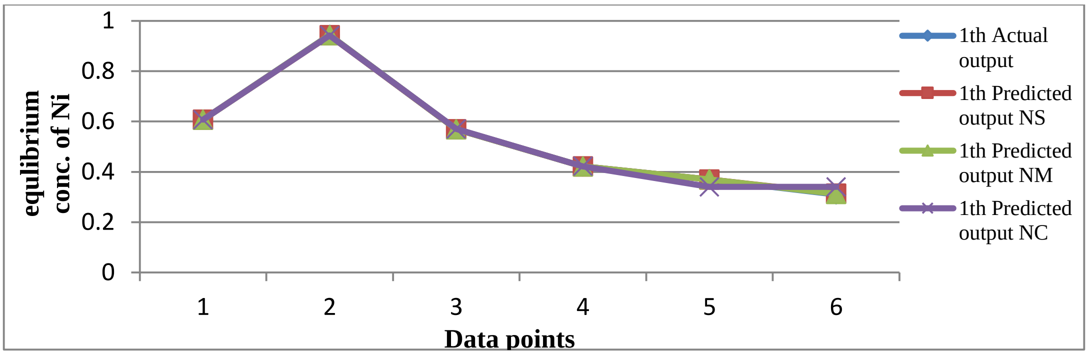

Figure 7. Comparison of actual and predicted values of equilibrium concentration of Ni(II) for training data set obtained using models NS, NM & NC

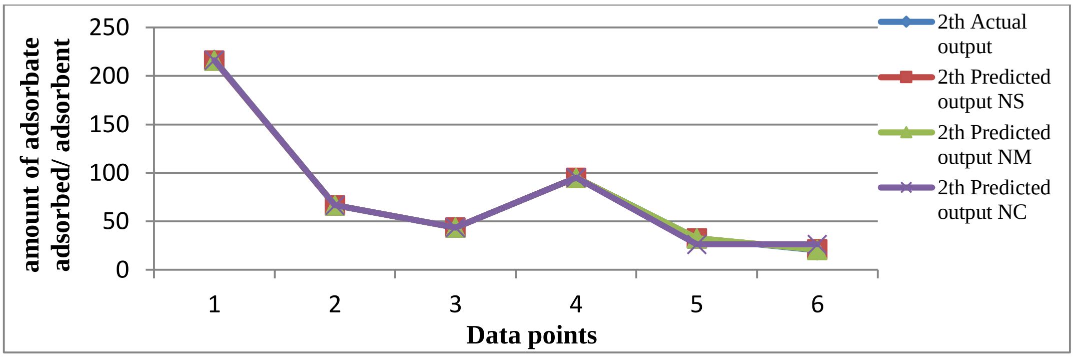

Figure 8. Comparison of actual and predicted values of amount of Ni(II) adsorbed/adsorbate for training data set obtained using models NS, NM & NC

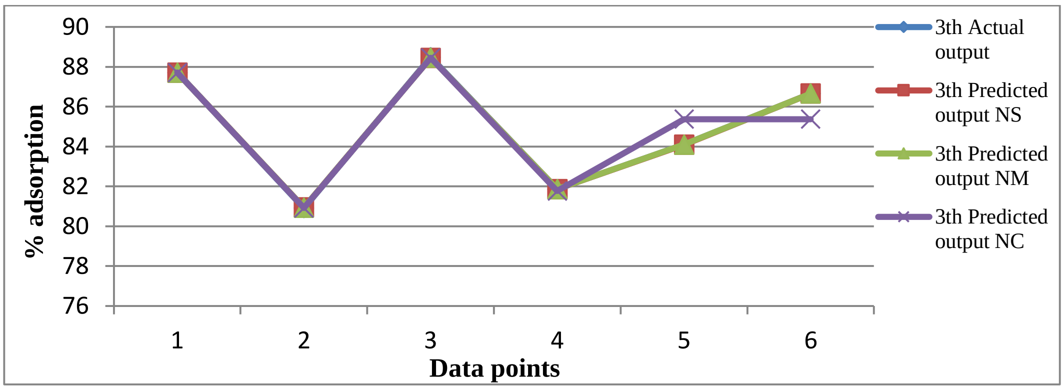

Figure 9. Comparison of actual and predicted values of % adsorption of adsorbates for training data set obtained using models NS, NM & NC

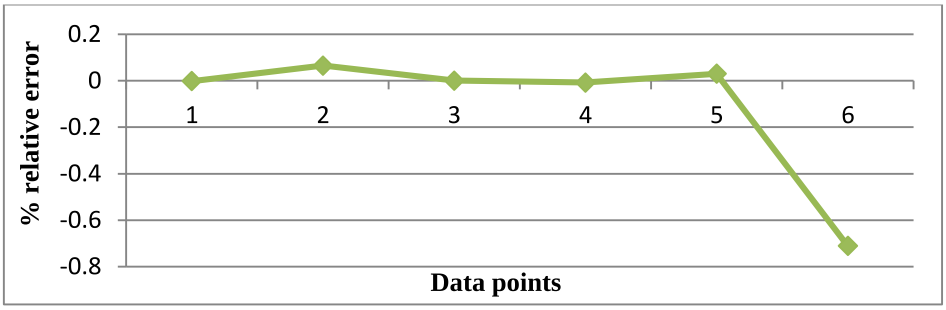

Figure 10. % Relative error for equilibrium concentration of Ni (II) for training data set obtained by model NM

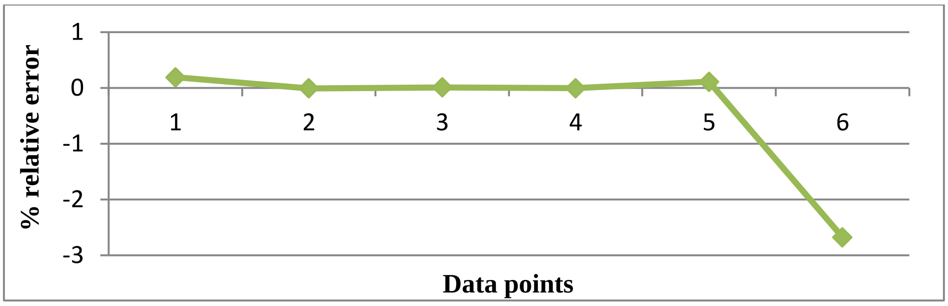

Figure 11. % Relative error for amount of Ni(II) adsorbed per unit adsorbent for training data set obtained by model NM

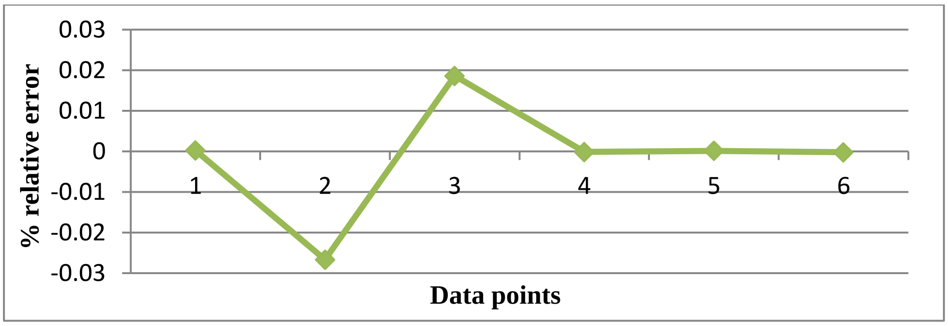

Figure 12. % Relative error for % adsorption of Ni (II) for training data set obtained by model NM

As can be seen from these figures the accuracy of prediction using NM model is ranged between 0 to 0.7%, 0 to -3% & 0 to 0.03% for equilibrium concentration of Ni(II) ions, amount of adsorbate adsorbed per unit amount of adsorbent and % adsorption respectively.
Accuracy of prediction is high & acceptable.

V. CONCLUSION & FUTURE SCOPE

The present work addresses towards the removal of Ni(II) ions from aqueous solution using aegel marmelos fruit shell adsorbent with various process parameters. The percentage adsorption is estimated in the range of 81-88%. It is observed that the percentage adsorption increases with the increase in adsorption dosage.
Based on the results & discussions it can be concluded that the present work has successfully addressed to the theme of application of ANN modeling in the adsorption studies related to the removal of Ni(II) ions from aqueous solution using Aegel Marmelos fruit shell adsorbent. Two ANN models S-1 & S-2 are developed for standardization of digital colorimeter for estimation of concentration of Ni(II) ions from aqueous solution and three ANN models NS, NM & NC are developed for the estimation of % adsorption & equilibrium concentrations of Ni(II) ions on solid & liquid phases as a function of feed concentration & adsorbent dosage successfully with high accuracy and can be used effectively. The ANN model NM having two hidden layer with ten neuron each is

observed to be best out of these three & the accuracy of prediction is ranged between 0 to 0.7%, 0 to -3% & 0 to 0.03% for equilibrium concentration of Ni(II) ions, amount of adsorbate adsorbed per unit amount of adsorbent and % adsorption respectively.

It is felt necessary that similar work should be extended and expanded to adsorption studies involving combinations of adsorbent & adsorbate. The highlight & the novel feature of the present work is the application of ANN modeling in estimation of concentration of Ni(II) ions present in aqueous solution based on the optical density of aqueous solution. This technique may prove to be effective, low cost and accurate method of analysis for aqueous solution containing heavy metallic ions.

The present study is indicative & representative of several possible applications of Artificial neural network modeling in the area of adsorption involving several combinations of adsorbent & adsorbates.

ACKNOWLEDGEMENT

Authors are thankful to Director, LIT, Nagpur for the facilities provided.

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