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Neural Network Modeling & Efficiency of Agro-Waste Charcoal for Removal of Non-Ionic Surfactant

Jyoti Kapil Nagwanshi[1], Manisha Agrawal[2], Amit Yerpude[3]
Research Scholar[1], Professor & Head[2], Applied Chemistry, Assistant Professor[3],
Computer Science and Engineering[3]
Rungta College of Engineering & Technology[1, 2&3], Kohka, Bhilai
Corresponding Authors: jyotikapiln@gmail.com[1], dr.manisha.agrawal@rungta.ac.in[2]

Abstract- This paper deals with the potential use of agro-waste material as adsorbent base for removal of non-ionic surfactant from wastewater. A single neural network (NN) model was applied to predict an array of percentage adsorption behavior of Triton X-100 (TX-100). A series of experimental data were collected and fitted with a unique NN model. Result shows that a single NN structure with 7 inputs, hidden layer having 10 neurons and 1 output are able to represent accurately the percentage removal of TX-100.

Agricultural wastes are low-cost adsorbents and can be viable alternatives to commercial activated carbon for treatment of surfactant-contaminated wastewater. Carbonized peels display better adsorption capacity. In the present investigation, the fundamental mechanism of surfactant adsorption characteristics on carbonized orange peel (COP) is studied by using spectrophotometric method. Equilibrium experimental data were fitted to the Freundlich, Langmuir and Temkin isotherm equations. Results show that Langmuir model fits the data better than any others, with relatively high R^2 value. In neural network programming, the R^2 value of overall validation reveals that single NN model can be applied in simulation and design with confidence.

Keywords- Adsorbent; Non-ionic surfactant; Neural network model; Spectrophotometric method.

1. INTRODUCTION

Surfactants or surface active agents are amphiphilic organic compounds, which are foaming and wetting agents that form the basis for most aqueous cleaners. Non-ionic surfactants, particularly TX-100 have been widely used in plating of metals, ingredient in influenza vaccine, in DNA extraction: parts of lysis buffer, dispersion of carbon materials for soft composite materials. Apart from laboratory use, it can be found in several kinds of cleaning products; ranging from heavy compounds to gentle detergents. It is also a popular component in homemade vinyl record cleaning fluid. It is a good micellar catalyst too. It is 100% active ingredient, which is often used in biochemical applications to solubilize proteins. It has no antimicrobial properties. Hence, it is considered as a comparatively mild non-denaturing surfactant. TX-100 [$C_{14}H_{22}O(C_2H_4O)_n$] is a representative of nonionic detergents, which is produced from octylphenol polymerized with ethylene oxide. The number “100” relates only indirectly to the number of ethylene oxide units in the molecular structure. TX-100 has an "average of 9.5" ethylene oxide units per molecule. It is an excellent detergent and dispersant, which is used as household and industrial cleaners. TX-100 is widely used in paints and coatings, textile industry, paper and pulp industry, agrochemical industry etc. TX-100 is used in different personal care products, which are shown in figure 1.

Fig. 1. Uses of TX-100 in Different Personal Care Products

Surfactants can be analyzed and eliminated from wastewater by several methods, such as-chromatographic techniques [1], spectrophotometric approach [2]; [3]; [4], potentiometric titration [5], flow injection analysis [6], voltametric technique [4], photodegradation under UV/H_2O_2 process [7]; [8], UVC Photolysis and advanced oxidation [9]; [8], anaerobic biodegradation [10]; [11]; [12], foaming, ozonation [13]; [14], nano-filtration [15], ultra-filtration [16]; [17], ion-exchange [18]; [15]; [16]; [17], coagulation process [19], HPLC coupled with universal mass etc.

Adsorption [20]; [21]; [22]; [23]; [24]; [25]; [26] process has advantages over above method in terms of initial cost, ease of operation, simplicity of design, less time consumption. It is a commonly used chemical engineering separation process, whereby two or more components of liquids are separated through contact with a solid surface. The process of adsorption is now viewed as a superior method for wastewater treatment and water reclamation.

2. MATERIALS AND METHODS

2.1 Reagents

EPA guidelines **[27]** were followed to prepare aqueous solutions of Merck made analytical reagent (AR) grade TX-100 and kept in air-tight bottles in refrigerator for further use.

2.2 Instruments/ Apparatus

Systronics PC Based Double Beam Spectrophotometer (Model-2202) was used to measure optical density (OD). Muffle furnace was used to prepare carbonized charcoal [28] from orange peels and used as non-conventional adsorbent. To calculate the percentage removal of TX-100, following Equation (1) was applied-

- % removal of TX-100 in effluent = $\frac{C_i \, x \, 100}{Residual\ concentration\ of\ TX-100}$ Eq. (1)

where, C_i = Initial concentration of TX-100

2.3 Experimental Protocol

The batch adsorption experiments were conducted for checking the capacity of fresh COP, acid activated recycled and alkali activated recycled COP.

2.4 Optimization of Experimental Conditions

Optimization is done by changing dose of adsorbent bed to check the efficiency of the bed by measuring OD and percentage removal of TX-100. Neural network modeling was performed to obtain the over-all performance and regression co-efficient values of the experiment. For getting accurate values, experiments were performed independently and repeated again and again.

2.5 Adsorption Isotherm

Adsorption isotherms were studied to estimate that the adsorbate is trapped onto the adsorbent in monolayer or multilayer pattern. In the current study three most popular adsorption isotherm models: Freundlich, Langmuir **[29]** and Temkin **[30]**; **[31]**; **[32]** were employed.

2.6 Neural Network Model

Neural networks have been the subject matter of significant research interest for the past twenty to twenty-five years. Artificial neural networks (ANNs) attempt to imitate how a biological system functions and how they can be utilized for their novel architecture. ANNs can simply be viewed as general non-linear models which have the ability to co-relate the relationship between a series of inputs and outputs of a system [33]; [34]. ANNs are now being used for a wide variety of engineering applications. They possess a high degree of flexibility that allows them to easily capture the nonlinear behavior of a process using input-output data.

A three layered neural network (NN) normally consists of- an input layer, a hidden layer and an output layer. The NN that has been used in the current study is presented in figure 2. The input layer receives the process inputs and fans out this information to all functional neurons of the hidden layer. Each neuron of the hidden layer essentially performs two tasks: (1) a weighted summation of all process inputs; and (2) a non-linear transformation, via a neuron transfer function, of the weighted summation to produce the output of each neuron of the hidden layer which then serves as inputs to the neurons of the output layer. The output layer performs the same task as the neurons of the second layer to produce the final output of the NN. The typical transfer functions that are used in the hidden and output layers are random.

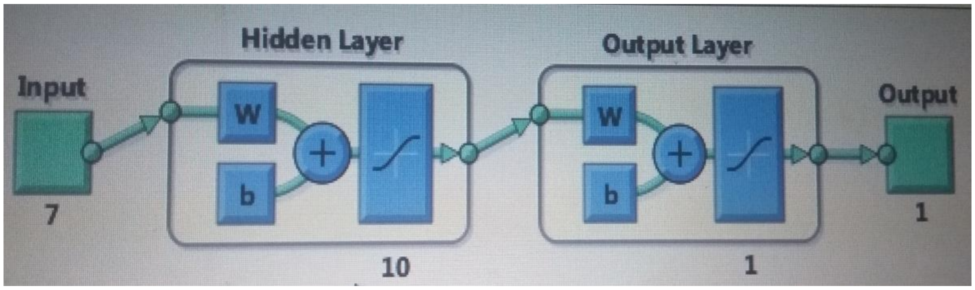


Fig. 2. Three Different Layers of Artificial Neural Network

3. RESULTS AND DISCUSSION

The OD and percentage removal of TX-100 parameters are plotted against different adsorbent bed dosages. Related figures are shown in figure 3 and 4.

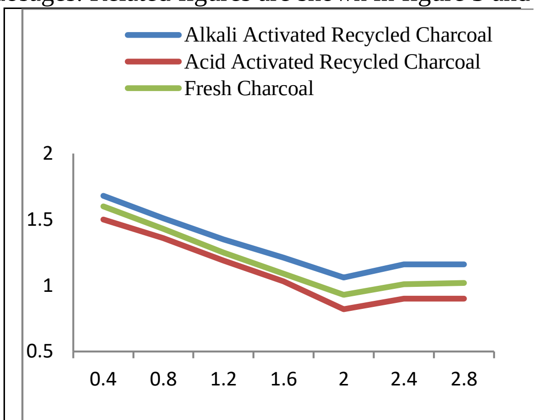


Fig. 3. A plot of adsorbent bed dose Vs OD

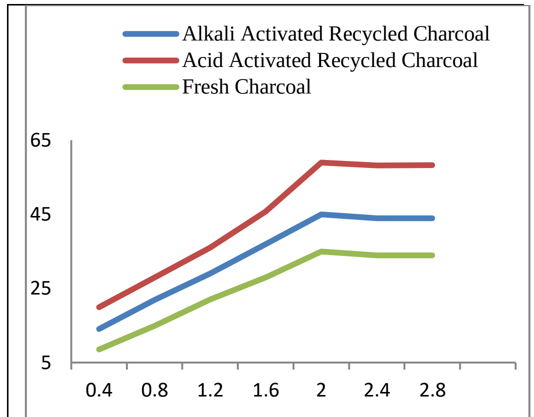
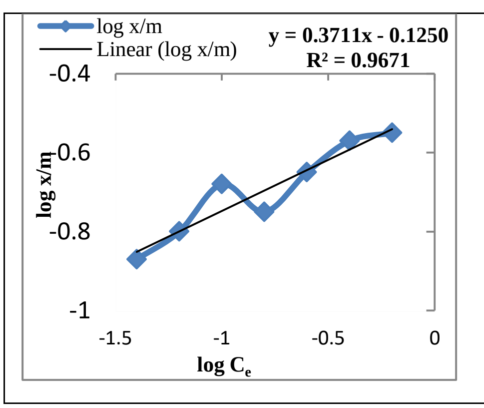
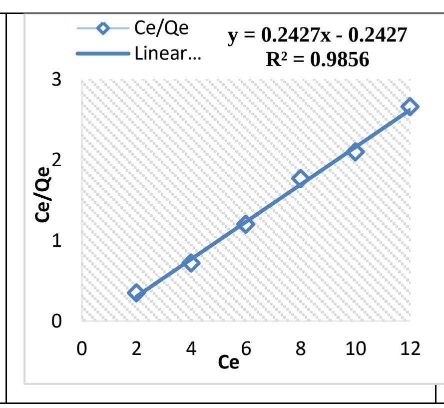


Fig. 4. A plot of adsorbent bed dose Vs % removal

Figure 3 is the plot of adsorbent bed dosage versus OD. Before adsorption, the concentration of TX-100 was larger. Thus the value of OD was high, but after adsorbing surfactant with 0.4 gm. to 2.0 gm. dosages, OD gets lowered. The reason is that up to 2.0 gm adsorbent bed dose, more and more TX-100 gets adsorbed and thus OD decreases. Equilibrium reached after 2.0 gm dose. Acid activated recycled COP gives better result than fresh charcoal and alkali activated recycled charcoal. Figure 4 is the plot of adsorbent bed dosage versus percentage removal. Acid activated recycled COP adsorbs highest amount of TX-100 as compared to fresh charcoal and alkali activated recycled charcoal. Equilibrium reached after 2.0 gm bed dose as the adsorption sites of bed get blocked by adsorbate molecules.

Three important equilibrium isotherm models-Freundlich, Langmuir [29]; [26] and Temkin [31]; [32]; [35] have studied. Related graphs are shown from figure 5 to 7.





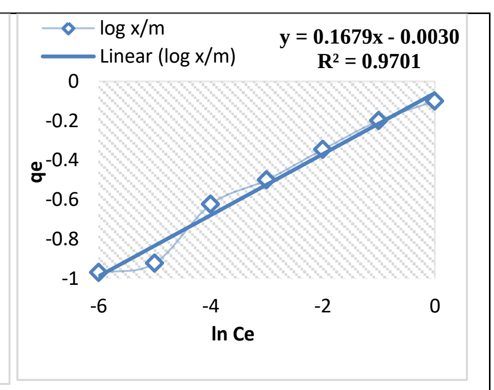


Fig. 5. A plot of Freundlich adsorption isotherm for adsorption of TX-100	Fig. 6. A plot of Langmuir adsorption isotherm for adsorption of TX-100	Fig. 7. A plot of Temkin adsorption isotherm for adsorption of TX-100

In neural network modeling, the result of best validation performance is shown in figure 8. At epoch seven, 93.62% performance is obtained.

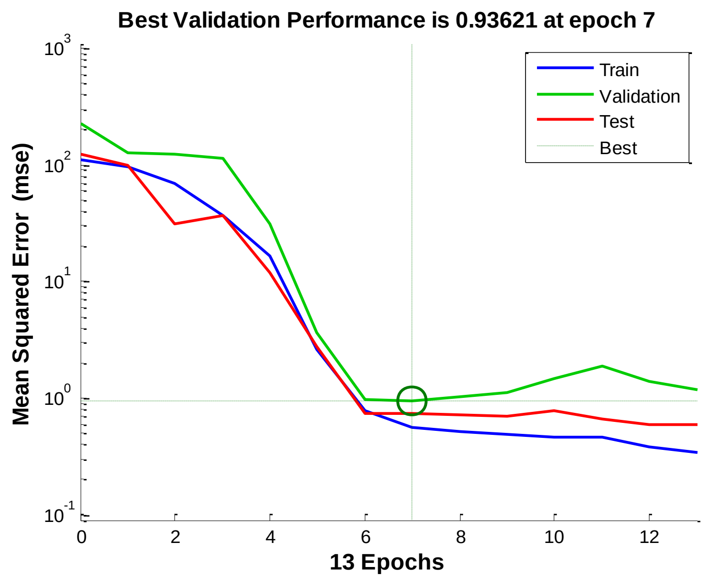


Fig. 8. A plot of best validation performance at epoch 07

The values of different regression co-efficient for training, validation, test and overall validation are shown in figure 9. The value of R^2 for overall validation indicates that the accuracy of the fit is truly excellent. As a result, one could use the neural network model with confidence in simulation and design.

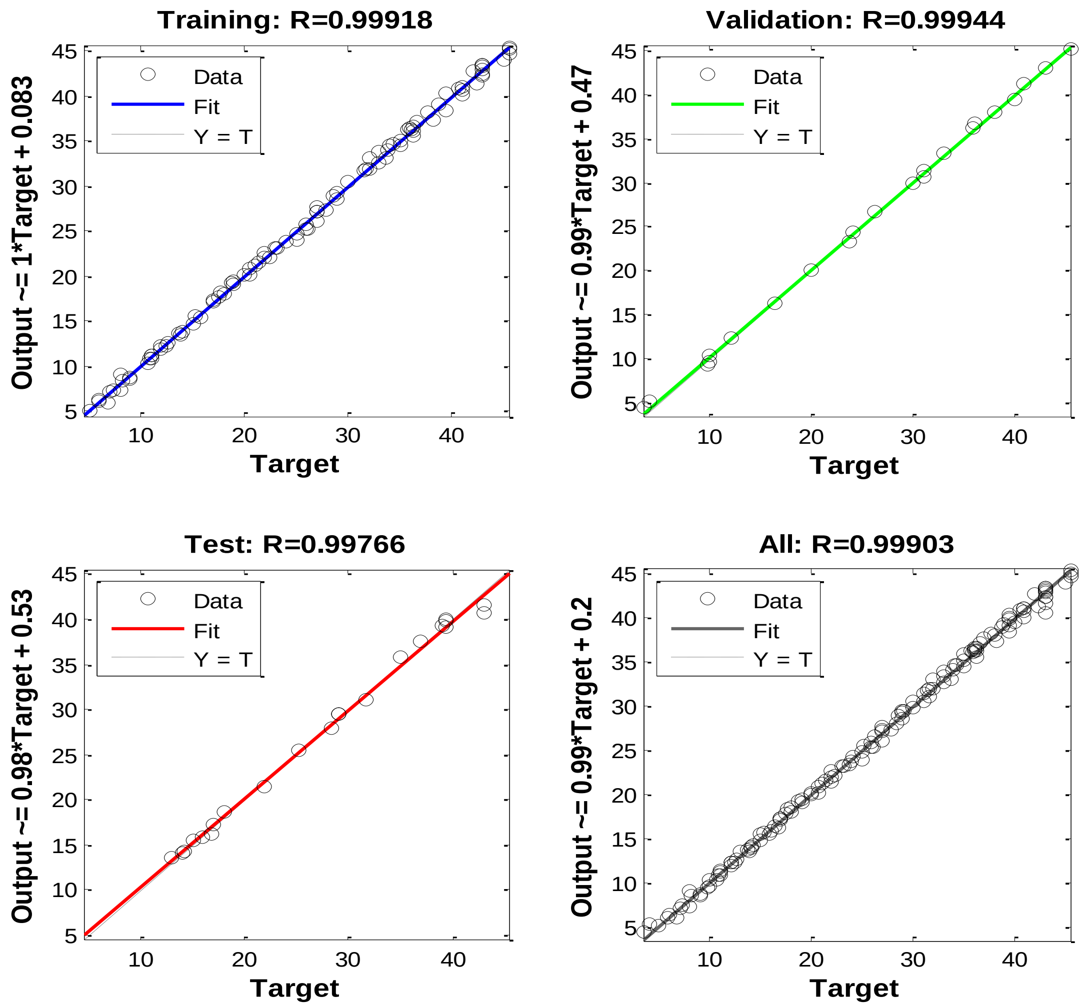


Fig. 9. Values of Regression co-efficient for different parameters

4. CONCLUSION

In this study, the ability of neural network is examined for its efficiency to represent a wide array of percentage adsorption behavior of data. It is found that the proposed model is highly effective to represent adsorption of TX-100 with the flexibility to exactly fit data. In addition to it, fresh charcoal, alkali activated recycled and acid activated recycled charcoal have compared and it is found that acid activated recycled charcoal is better adsorbent bed than fresh and alkali activated recycled charcoal. Linear regression co-efficient (R^2) values of Freundlich, Langmuir and Temkin adsorption isotherms are 0.9671, 0.9856 and 0.9701 respectively. The adsorption data fits into all the three models, out of which Langmuir model is found to be have the highest R^2 value and hence the best fit. Adsorption has been proven to be a potential advanced physicochemical treatment method for the effective removal of non-ionic surfactant present in effluent intended for reuse. Carbonized orange peel charcoal is used as effective agro-waste adsorbent bed, in the way of removing TX-100 through adsorption. Even after use for adsorbing surfactant, this bed can be reused as domestic fuel. This can also be used as additive with conventional beds with no side effects. It may be a better replacement of synthetic adsorbent beds. Results of the study demonstrate usability of agro-waste charcoal as a promising adsorbent base in surfactant adsorption. The use of artificial neural networks is wide to analyze the data and to control dynamic processes. These tools are powerful and versatile. ANNs offer an analytical option to conventional techniques, which are often limited by strict assumptions of linearity, normality, variable independence etc. Since an ANN can capture many kinds of relationships, it allows the user to rapidly and comparatively easily model phenomena, which otherwise may have been very difficult or impossible to explain otherwise.

The use of low-cost agro-waste adsorbent is recommended since it is relatively cheap or of no cost, easily available, renewable and shows highly affinity for surfactant. The process of adsorption requires further investigation in the direction of modeling, regeneration of adsorbent and immobilization of the waste material for improved efficiency and recovery. Furthermore interest should be generated by the researchers to predict the performance of the adsorption process for surfactant removal from real industrial effluents.

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