Wastewater treatment by adsorption process on mineral activated carbon: modeling and prediction using an intelligent artificial approach

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Abstract. Currently there are several wastewater treatments processes, and several adsorbent materials consist of separating and purifying the various industrial effluents. In this work an artificial neural network (ANN) was developed to describe the dynamic adsorption of sodium decanesulfonate using activated carbon obtained by the calcination of mineral biomass under different conditions. Three inputs (time, mass of adsorbent and fixed bed height) were used in the input layer, three neurons in the hidden layer and one in the output layer for the reduced concentration. The Levenberg Marquardt back-propagation algorithm was applied. The tangent sigmoid and linear transfer functions are used for the hidden layer and the output layer respectively. The results showed a correlation coefficient $R^2 = 0.9965$ with root mean squared error $RMSE = 0.0276$. An interpolation and an extrapolation stage are made to test the accuracy of the network. The results showed a high correlation coefficient $R^2 = 0.9969$ and 0.984 respectively for the interpolation and the extrapolation. These results show the robustness and the high capacity of ANN to describe the dynamic adsorption of sodium decanesulfonate onto actived carbon.

Keywords. Water treatment, fixed bed adsorption, Mineral biomass, Modelling, Artificial Neural Network.

1. Introduction

Water bodies are the most common natural resources that have been contaminated as a result of different human activities [1]. These wastewaters containing toxic compound coming from different industries had a harmful impact on the atmosphere and their reject has dangerous results can be lethal to the aquatic life and affecting directly on the ecosystem equilibrium for that they must be treated properly before their discharge to the environment [2,3].

Adsorption has been extensively studied by researchers worldwide as an efficient and economically sustainable technology for the treatment of effluents [4].

Fixed bed adsorption or dynamic adsorption is widely used for purifying liquid mixtures, especially industrial waste effluents. This technical is more appropriate due to its low cost and high efficiency [5,6]. Artificial neural networks (ANN) are computational models as set of algorithms; they resemble the human brain [7]. They are now used as a very powerful tool to model nonlinear systems and they are considered more reliable than other mathematical models because they have a high parallelism and a high robustness [8, 9].
The ANN architecture containing a number of hidden layers, input layer (independent variables), and output layer. Each of these layers consists of a number of interconnected processing units called neurons. These neurons are connected between them by links or weights [10].

Several works have used ANN as a black box to predict the dynamic adsorption phenomena.

(Kittisupakorn P et al.) [11] developed an artificial neural network to predict the dynamic adsorption of Hydrochloric Acid onto Ion Exchange Resin. (Celekli A et al.) [12] studied the removal modeling of Lanaset Red G on Chara contraria by ANN. (Sediri M et al.) [13] in their work, they developed an ANN to predict the fixed bed adsorption of p-nitrophenol onto NDA-100 resin.

The aim of this work is to develop an artificial neural network (ANN) to predict the dynamic adsorption of sodium decansulfonate onto activated carbon under different conditions. The accuracy of the optimal network obtained was tested by studying the interpolation and the extrapolation performance.

2. Materials and methods

2.1. Materials

The system (adsorbate/adsorbent) studied in this work was the Sodium decanesulfonate/activated carbon. Experimental data points were taken from the article of Sahel and Ferrandon-Dusart [14], and arranged as matrix containing 156 experimental data points. The activated carbon properties are shown in Table 1.

| Characteristic          | value |
|-------------------------|-------|
| Area surface (m²/g)     | 1100  |
| Particle diameter (mm)  | 1     |
| Apparent density (kg/m³)| 535   |

2.2. Methodology

The feed-forward back propagation neural network (FFNN) with Levenberg Marquardt back-propagation Learning algorithm is one of the most famous neural network paradigms used in the modeling of non-linear systems which has been used in our study. For the training/testing of the FFNN-LMBP, 156 experimental data points were collected and arranged as matrix of dimension of (156, 4).
Three (03) parameters (time (t), mass of adsorbent (m) and fixed bed height (H)) were used as inputs in the input layer of the ANN and the reduced concentration (C/C₀) selected as the output parameter in the output layer. The ANN architecture is shown in Fig.1.

The normalization of the experimental data in the interval [-1, 1] was achieved using the mapminmax function given by the following equation [15]:

\[
X_{\text{norm}} = Y_{\text{min}} \left( \frac{X_i - X_{\text{min}}}{X_{\text{max}} - X_{\text{min}}} \right) \left( Y_{\text{max}} - Y_{\text{min}} \right)
\]

Where \( X_i \) is the input or output variable X, \( X_{\text{min}} \) and \( X_{\text{max}} \) are the minimum and maximum values of variable X, \( Y_{\text{max}} = +1 \), \( Y_{\text{min}} = -1 \).

The splitting of the experimental data was also achieved into three phases: training, validation and testing phase. For the hidden layer the number of neurons was changed from 1 to 10. The tangent sigmoid (tansig) and linear (purelin) activation function used at hidden and output layer respectively.

The performances of the neural network were calculated using the root mean square error (RMSE) and correlation coefficient (R²) given by the following equations [13,16]:

\[
R^2 = 1 - \frac{\sum_{p=1}^{p} \left( \frac{C}{C_0} \exp - \frac{C}{C_0} \text{predict} \right)^2}{\sum_{p=1}^{p} \left( \frac{C}{C_0} \exp \right)^2}
\]

\[
\text{RMSE} = \left( \frac{1}{p} \sum_{q=1}^{p} \left( \frac{C}{C_0} \exp - \frac{C}{C_0} \text{predict} \right)^2 \right)^{1/2}
\]

Where, \( q \) is the number of data points, \( \frac{C}{C_0} \exp \) is the experimental reduced concentration and \( \frac{C}{C_0} \text{predict} \) is the predicted reduced concentration by the ANN model.

### 3. Results and discussion

#### 3.1. ANN developed model

In order to determine the optimal structure of ANN, the number of neurons was changed at hidden layer from 1 to 10 using the tansig activation function. Each topology was repeated three times. According to the values of correlation coefficient (R²) and root mean square error (RMSE), three neurons are obtained at hidden layer corresponds to the agreement vector \([ R^2 , \text{RMSE} ]\) approaching to the ideal \([ R^2=1, \text{RMSE}=0 \] \). Fig .2 shows the comparison between experimental and predicted data by ANN model. This plot has \( R^2 = 0.9965 \) and RMSE= 0.0276 provide the reliability of the developed ANN model.
Figure 2. Comparison between calculated values by ANN and experimental values

The breakthrough curves of sodium decanesulfonate as a function of time under different conditions were depicted in Fig. 3. The experimental data points are very approaching to those obtained by the ANN, which shows the robustness of neural network model.

Figure 3. Breakthrough curve of sodium decanesulfonate onto activated carbon, \(C_0=20\text{mg/l}, \text{flow rate } Q=0.435\text{l/h} \)
3.2. Interpolation performance

An interpolation was studied to check the precision of the ANN model developed. A database was used containing a set of data points situated at the intermediate of the experimental points of a breakthrough curve of sodium decanesulfonate / activated carbon system. The results of interpolation performances in terms of error (RMSE) and agreement vector values [\(\alpha\) (slope), \(\beta\) (y intercept), \(R^2\) (correlation coefficient)] are presented in Table 2. The plot of breakthrough curve of interpolated experimental data and predicted data is shown in Fig.4. These results showed the robustness of ANN developed model.

| Interpolation performances | RMSE | \(R^2\) | \(\alpha\) | \(\beta\) |
|----------------------------|------|---------|-------|-------|
|                            | 0.0274 | 0.9969 | 0.98  | 0.01  |

Figure 4. Simulation results of interpolation: \(C_0=20\)mg/l, flow rate \(Q=0.435\) l/h, \(H=4\)cm, \(m=3\)g.

3.3. Extrapolation performance

An extrapolation was also studied to check the accuracy of the ANN model developed. For that we have testing an experimental data point never exploited during the learning and the testing phases of ANN previously developed. Results of extrapolation performances were showed in Table 3. Fig. 5 showed the breakthrough curve of extrapolated experimental data with those obtained by ANN. The results provide that the ANN model predicts the experimental data very well.
Table 3. Extrapolation results in terms of error (RMSE) and vector $[\alpha, \beta, R^2]$.

| Extrapolation performances | RMSE | $R^2$ | $\alpha$ | $R$ |
|-----------------------------|------|-------|---------|-----|
|                             | 0.0745 | 0.984 | 0.91    | 0.019 |

![Extrapolated experimental data](image)

Figure 5. Simulation results of extrapolation: $C_0=20\text{mg/l}$, flow rate $Q=0.435\text{ l/h}$, $H=3.10\text{cm}$, $m=2.33\text{g}$.

4. Conclusion

An ANN was developed in this work to predict the dynamic adsorption of sodium decanesulfonate using activated carbon as adsorbent. For this purpose, three neurons were used in the input layer, three in the hidden layer with tansig activation function and one neuron is used in the output layer with purelin activation function. Levenburg-Marquardt learning algorithm was applied. The results showed a high correlation coefficient of order of 0.9965 with root means square error close to 0.

The high correlation coefficients obtained of 0.9969 and 0.984 values for the interpolation and for the extrapolation stage respectively showed the accuracy and the robustness of the neural network developed model.

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