Journal of Materials and Environmental Sciences
ISSN : 2028-2508

JMES, 2017 Volume 8, Issue 7, Page 2282-2287

http://www.jmaterenvironsci.com /

ERVD4, 26-27 Oct 2016 Ifrane, Morocco

Dynamic Adsorption Modelling of P-nitrophenol in Aquous Solution Using Artificial Neural Network

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Received 04 Jul 2016,
Revised 24 Aug 2016,
Accepted 01 Sep 2016

Keywords
- ✓ Dynamic adsorption,
- ✓ P-nitrophenol,
- ✓ NDA-100 resin,
- ✓ Modeling ,
- ✓ Artificial Neural Network.

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Abstract

This work aims at developing an artificial neural network to describe the dynamic adsorption of p-nitrophenol from an aqueous solution using an NDA-100 resin as adsorbent under different conditions. Nine neurons were used in the input layer corresponding to the nine input parameters (time, area surface, particle diameter, mass of adsorbent, bed high, apparent density, molar mass, initial concentration and flow rate) and one neuron in the output layer corresponds to the reduced concentration. After training/test and validation, the best ANN was found with four neurons in the hidden layer with the transfer function (tangent sigmoid), Levenberg Marquardt retro-propagation algorithm and linear transfer function for the output layer. The optimized ANN was obtained with a high correlation coefficient of R^2 = 0.9992 and mean squared error of MSE = 0.00028 during the generalization phase. An interpolation and a prediction stage have been done to test the reliability of the best ANN. Results obtained from the interpolation gave a correlation coefficient of R^2 = 0.999 and mean square error MSE = 0.00036, so for the prediction are R^2 = 0.9187 and MSE = 0.0478. These results show that the proposed ANN model is able to accurately predict the reduced concentration of the dynamic adsorption phenomenon of p-nitrophenol using an NDA-100 resin.

1. Introduction

The increase in the number of industrial sites and human activities has had a negative impact on the environment, due to the large quantities of toxic species generated and emitted in nature, in different states: gaseous, solid or liquid. This is a major concern for public authorities because of the possible consequences on living species and their environment as well as for the following two main reasons: the great variety of metals and the large number of chemical combinations to which they can thus participate by the toxic effects they may cause [1].

Phenolic products are among the most harmful organic components on the environment, even at very low concentrations due to its toxicity, nauseating odor and carcinogenic properties [2]. For this they must be treated before being released into the environment using a technological separation process. There are several technological methods that serve to treat and reduce the pollutant load in effluents, we can mention (precipitation, membrane filtration, adsorption, photo-degradation, biodegradation, irradiation, and ozonation) [3]. In recent years, adsorption has been widely studied by scientific researchers as an efficient way to treat industrial waste, it is classified into two types: static and dynamic [4].

Dynamic or fixed bed adsorption is one of the most widely used techniques for separation and purification of effluents due to its low cost, high efficiency and easy operation. This technique usually occurs in an open system where the solution of the adsorbate passes through a column containing an adsorbent [4].

Dynamic adsorption modeling using Artificial Neural Networks (RNA) as an intelligent approach for simulation and system performance prediction is gradually becoming more and more popular in recent years. These networks are more reliable compared to conventional mathematical models because of their high parallelism, robustness and their ability to handle complex relationships between input parameters and output parameters of a process [5-7]. Several works have been carried out on the ANN: Chowdhury et al (2013) studied the dynamic adsorption of methylene blue by NaOH-modified rice husk in a fixed-bed column system [8]. In their work,

Tovar-Gomez et al (2013) studied the dynamic adsorption of fluoride on bone char using a hybrid neural network approach [9], Chakraborty et al (2013) studied the modeling of dynamic adsorption of crystal violet from aqueous solution using citric-acid-modified rice [10]. In the work of Meriem Sediri et al (2017) entitled : Artificial Neural Networks Modeling of Dynamic Adsorption From Aqueous Solution, they use multilayered perceptron artificial neural networks (MLP-ANN) and multiple linear regressions (MLR) models to predict the dynamic adsorption of the complex system of adsorbent-adsorbate in solid-liquid phase. They provide the superiority of MLP-ANN in prediction of adsorption and it gave more satisfactory results compared to the MLR model [11].

A neural network (RNA) was developed in this work to predict the dynamic adsorption of p-nitrophenol from an aqueous solution using an NDA-100 resin under different conditions. Then the reliability of our model was tested using an interpolation and a prediction. The calculations of the correlation coefficients and the mean squared errors were carried out.

2 .Artificial neural networks

Artificial neural networks (ANN) are a set of algorithms the design of which is at the origin very schematically inspired by the functioning of biological neurons. They are now used as a very powerful tool to model and analyze processes as well as to make the prediction of the behavior of a given system [5].

The ANN structure consists essentially of input layer (independent variables), a number of hidden layers and an output layer. Each of these layers consists of a number of interconnected processing units called neurons. These neurons interact by sending signals and they are connected to all the neurons on the previous layer, and the next layer by links called weights and links [12]. The architecture of the ANN model is showed in Figure. 1.

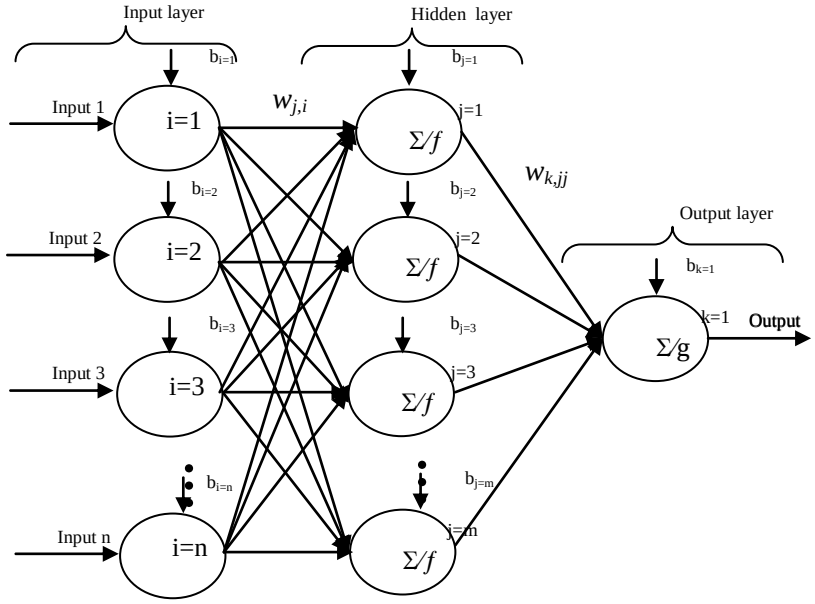

Figure1: Structure of ANN.

3. Materials and methods

3.1 Materials

The adsorbent studied is the NDA-100 resin whose properties had been taken from the paper of Pan-BC et al (2005) [13]. The NDA-100 resin properties are shown in table 1.

Table 1 : Proprerties of NDA-100 resin

Area surface (m^2/g)	721.5
Particle diameter (mm)	0.75
Apparent density (kg/m^3)	321.9

The adsorbate studied is p-nitrophenol the properties of which had been determined from article of Pan-BC et al (2005) [13]. The characteristics of p-nitrophenol are shown in Table 2.

Table 2 : Caracteristics of p-nitrophenol

Brute formula	$C_6H_5NO_3$
Molar mass	139.11
Wave lengh	318
Pka	7.16 (in water)

3.2 Methodology

The size of the database was arranged as matrix with (118,10) containing 09 inputs parameters (time (t), The specific surface area of the resin (As), particle diameter of resin (dp), mass of resin (m) , bed height (H), density of resin(ρ), molar mass of p-nitrophenol (M), initial concentration (C_0), flow rate (Q)) and an output parameter is the reduced concentration (C/C_0) of p-nitrophenol.
The experimental data were normalized in the interval [-1,1] using the mapminmax function as follows [14]:

$$X_{norm} = 2\left(\frac{X_i - X_{min}}{X_{max} - X_{min}}\right) - 1 \quad (1)$$

X_i is the input or output variable X, and X_{min} and X_{max} are the minimum and maximum values of variable X.

These data were divided into three phases: learning phase, test phase and validation phase. The number of neurons used in the input layer is 09 and for the output layer is 01.
In order to obtain an optimal neural network giving approximate results to the experimental data, a hidden layer was used by changing the number of neurons from 1 to 10. The Levenberg Marquardt retro-propagation algorithm was applied. The tangent sigmoid (tansig) and linear (purelin) transfer functions were used respectively for the hidden layer and the output layer.
The learning of the model must be done; each topology has been repeated three times. The optimal structure corresponds to the correlation coefficient R^2 close to 1 and means squared error MSE close to 0. The relations of R^2 and of MSE are given by the following equations [5, 15]:

$$R^2 = 1 - \frac{\sum_q^p \left[\left(\frac{C}{C_0}\right)_q^{exp} - \left(\frac{C}{C_0}\right)_q^{predict}\right]^2}{\sum_q^p \left[\left(\frac{C}{C_0}\right)_q^{exp} - \left(\frac{C}{C_0}\right)_n\right]^2} \quad (2)$$

$$MSE = \frac{1}{p}\sum_{q=1}^{p}\left[\left(\frac{C}{C_0}\right)_q^{exp} - \left(\frac{C}{C_0}\right)_q^{predict}\right]^2 \quad (3)$$

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

A MATLAB program is developed to perform the neural network development procedure.

4. Results and discussion

4.1 RNA developped model

According to the previous discussion, an artificial neural network is developed to predict the adsorption of p-nitrphenol in a fixed bed. Four neurons in the hidden layer were sufficient to achieve a better correlation coefficient (R^2) with a very small mean squared error (MSE). The results obtained are presented in Table 3 and in Figure 2.

Table 3: Optimal neural network structure

Training Algorithm	Input layer	Hidden layer		Output layer	
	Nomber of neurons	Nomber of neurons	Activation function	Nomber of neurons	Activation function
Levenberg-Marquardt Back-propagation	09	04	Tangent sigmoïde (tansig)	01	Linear (purelin)

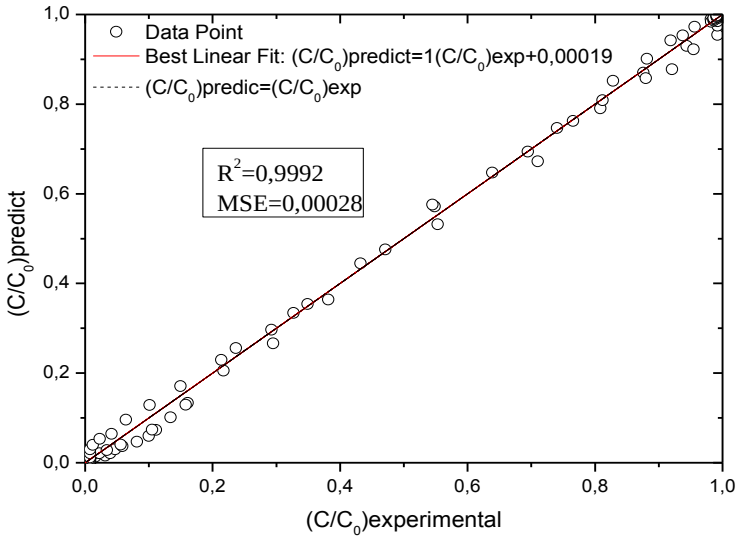

Figure 2 : The regression curve represents the predicted reduced concentrations depending on the experimental reduced concentrations.

These results show that there is a very good correlation between the predicted values and the experimental values with a better correlation coefficient R^2 = 0.9992 and better mean square error MSE = 0.00028, which shows the robustness of the established of neural model. The breakthrough curves of p-nitrophenol representing the comparison between the experimental results and those obtained by the ANN under different conditions as a function of time which are shown in Figure 3. We notice that the points of the experimental data are very close to those predicted by the ANN, which shows the reliability and the robustness of our developed model.

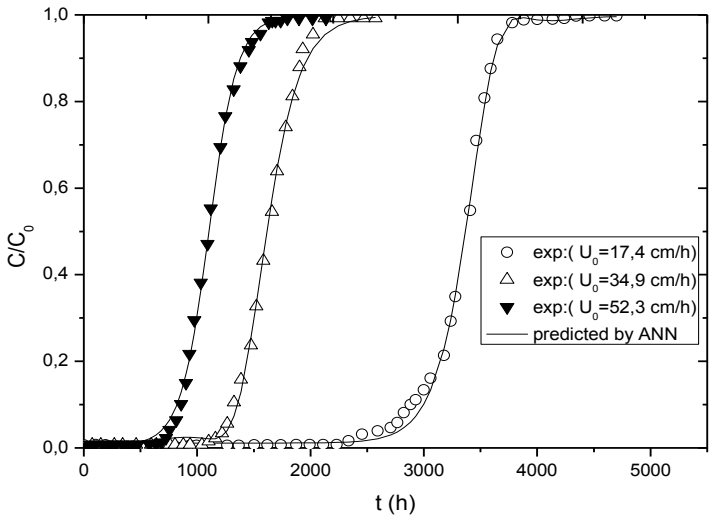

Figure 3: breakthrough curve of p-nitrophenol dynamic adsorption onto resin NDA-100 (C_0 = 5.32 mmol/l, H = 5.71 cm, H/D = 3.88, m=3 g).

4.2 Interpolation performance

In order to test the precision of the RNA model previously developed and optimized, an interpolation was performed. For this purpose, a data base was constructed containing a set of data points located at the middle between the experimental points of a breakthrough curve of p-nitrophenol-NDA-100 resin.

The results showing the regression curve between the predicted and experimental values and the performance of the interpolation in terms of error and correlation coefficient are shown in Figure 4.

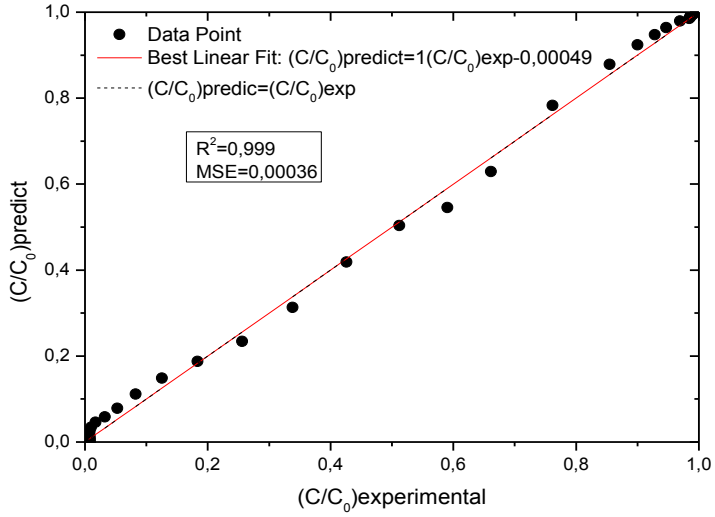

Figure 4: Regression curve of predicted reduced concentrations depending on the reduced experimental concentrations for interpolation.

These results show a good correlation between the predicted RNA and experimental values with a high correlation coefficient (R2 = 0.999) with a minimal error (MSE = 0.0036), which shows that our network is reliable and able to describe the dynamic adsorption phenomenon.

4.3 Prediction performance

Prediction is also performed to test the accuracy of our artificial neural network developed. The idea is to test points of an experimental data of another adsorbate / adsorbent system that has not been exploited during the learning of our network. The system therefore studied for this stage is phenol / resin NDA-100. The results in Figure 5 show a sufficient coefficient (R^2 = 0.9187) and a small error (MSE) of the order of 0.0478. This shows a good convergence between the experimental output and the output predicted by the RNA.

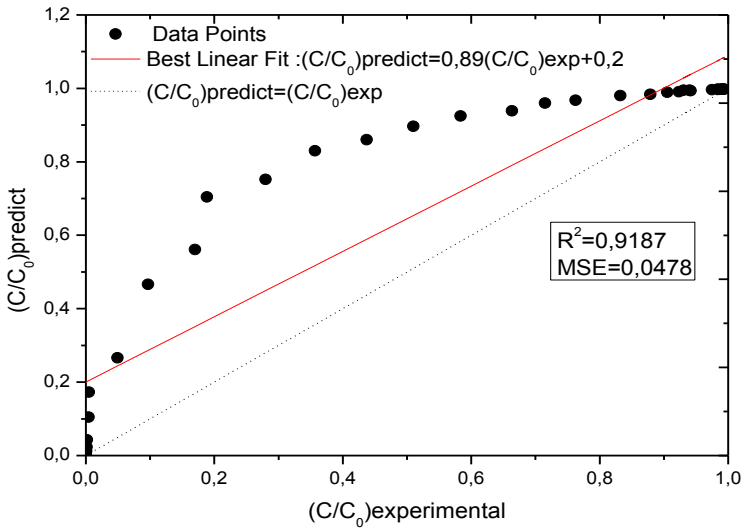

Figure 5: The regression curve of predicted reduced concentrations depending on the reduced experimental concentrations for the prediction. (U_0 = 34.9 cm/h, H = 5.71 cm, C_0 = 2.032 mmol/l,H/D = 3.88, m=3 g).

Conclusions

The goal of this study is to develop an artificial neural network in order to predict the dynamic adsorption of p-nitrophenol using an NDA-100 resin.

In order to have an optimal ANN giving good modeling, we used :

- 09 neurons in input layer.
- 04 neurons in hidden layer with tangent sigmoïde activation function.
- 01neuron in output layer with linear (purelin) activation function.
- Levenburg-Marquardt learning apprenticeship was applied

The obtained results are:

- Global correlation coefficient l R^2=0.9992 with mean square error MSE=0.00028
- The interpolation and prediction have proved the reliability of our network. The results show good correlation coefficients of the order of 0.999 and 0.9187 respectively for interpolation and prediction with mean squared errors close to 0.

These results show that the proposed model is able to accurately predict the reduced concentration of the dynamic adsorption phenomenon of p-nitrophenol using an NDA-100 resin.

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