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Representation of Adsorption Data for the Case of Energetically Heterogeneous Solid Surfaces Using Artificial Neural Network

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Abstract
In this study, adsorption data for the case of energetically heterogeneous solid surface are modeled using artificial neural network. A neural network with three hidden neurons, including the bias, was able to predict very accurately the temperature dependency of adsorption data. The results were compared with experimental data (over temperature range 273-313 K and 0-2 MPa pressure) and it was found that the predictions of the artificial neural network model fit the experimental data very accurately.

Keywords: *Artificial Neural Networks, Heterogeneous Solid Surfaces, Adsorption*

1. Introduction
Adsorption phenomena have been known to mankind for a very long time, and they are increasingly utilized to perform desired bulk separation or purification purposes. It is a process whereby two or more components of a fluid (gas or liquid) stream are separated through contact with a solid surface. The temperature and the composition (partial pressure or concentration) as well as various physical and chemical properties of the adsorbate-adsorbent pair affect the quantity of the component which can bind to the surface of the adsorbent.

It is well known that the real surfaces are energetically disordered to a larger or smaller extent. It shows the variation of adsorption energy when going from one site to another site on the surface. The contribution of solid toward heterogeneity is the geometrical and energetical characteristics, such as the micropore size distribution and the functional group distribution. In the case of activated carbons the geometrical porosity is the result of differences in the size and shape of pores as well as pits, vacancies, etc. Chemical heterogeneity is associated with different functional groups on the surface [1].

Over the years, many adsorption isotherm systems have been modeled using particular equations such as Freundlich, Langmuir, Toth, Sips, and isotherm models among others. Although these classic adsorption isotherm models are capable of showing

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certain equilibrium data sets by themselves, they also exhibit a considerable lack of fit when modeling non-traditional systems. The variable nature of these adsorption isotherms presents a challenge to the development of an equation that can be used to model the behavior of all adsorption systems. For example, Padmesh et al. [2] applied a total of ten different isotherm equations in an attempt to find an appropriate equation that will fit their adsorption data. To date, a single unifying equation to model all types of adsorption isotherms has yet to be constructed.

Feedforward neural networks have been successfully used in many usages associated with adsorption. It was used in the simulation and optimization of a pressure swing adsorption process for the separation of nitrogen from air [3]. Carsky and Do [4] predicted the adsorption equilibrium of binary vapor mixtures on activated carbon. Basu et al. [5] used a neural network to predict the effect of temperature on equilibrium adsorption of hydrocarbon gases and vapors on activated carbon. Mjalli et al. [6] used neural networks to represent the adsorption data for isopropanol-water system. Giraudet et al. [7] modeled with a neural network the heat of adsorption from volatile organic compound molecular properties and physical characteristics of activated carbons. Vasina et al. [8] used neural networks to represent protein adsorption. For predicting the equilibrium data of hydrogen onto activated carbons, Kumar et al. [9] used a three-layer feed-forward artificial neural network.

The present study is aimed to show the ability of neural network to describe adsorption data in different experimental conditions for the case of energetically heterogeneous solid surfaces. A neural network with three hidden neurons, including the bias, was used to predict very accurately the temperature dependency of adsorption data and the results show that unique neural network model fit each experimental data very accurately.

2. Artificial neural network (ANN)

Artificial neural networks are highly flexible mathematical constructs that have been inspired by the workings of the biological nervous system. ANNs have a natural tendency for storing experiential knowledge and making it available for use [10]. ANNs can simply be viewed as general nonlinear models which have the ability to encapsulate the underlying relationship that exists between a series of inputs and outputs of a system.

There are many different ANN structures like MLP (multi layer perception), RNN (recurrent neural network) and RBF (radial basis function). Each of these structures has been used for modeling different case studies.

Feedforward neural networks (FFNN) are undoubtedly the most common neural network structure used in engineering applications. It has been shown that a three-layer FFNN can represent any function provided that a sufficient number of neurons is present [11]. A FFNN normally consists of three layers: an input layer, a hidden layer, and an output layer. The feedforward neural networks that have been used in this examination are presented in Fig. 1.

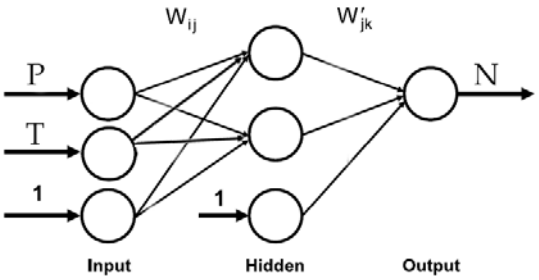

Figure 1. Feedforward neural networks used to represent temperature-dependent isotherm data sets

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 accomplishes 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 serve 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 FFNN. The typical transfer functions that are used in the hidden and output layers are linear, sigmoid or hyperbolic tangent. The input and output to the FFNN are usually scaled between 0 and 1.

3. Results and discussion

The ultimate goal of this investigation was to test the ability of simple artificial neural network structures with the least number of parameters to represent a wide variety of adsorption data for the case of energetically heterogeneous solid surfaces.

Experimental equilibrium isotherms for C_2H_6, C_3H_8 and CH_4/Ajax activated carbon are measured by Qiao and Hu [12]. The CH_4 and CO_2/activated carbon measured by Buss [13] were fitted using the neural network architecture of Fig. 1 with three hidden neurons, including the bias, because with four hidden neurons, better predictions were obtained for the learning data set but a weaker predictive ability of the neural network for the validation data set was observed, thereby indicating that over fit prevailed. This neural network consists of two independent variables (the adsorbate fluid pressure, *P*, and temperature, *T*) and one dependent variable (the adsorbate solids concentration, *N*). Figs. 2–6 present the results obtained for the four series of adsorption data.

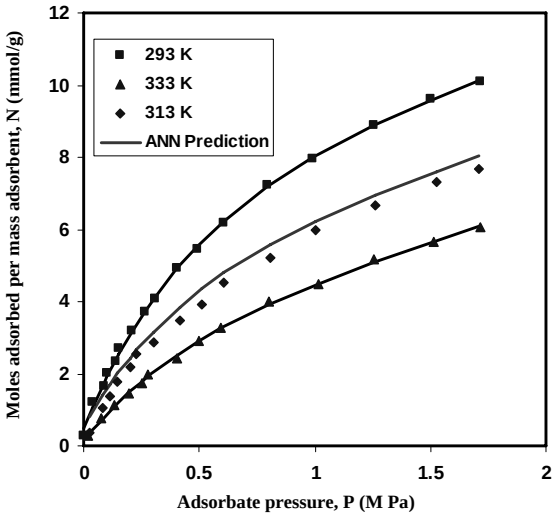

Figure 2. Comparison of the experimental adsorption data for CO_2/activated Carbon measured by Buss[13] with ANN(solid line)

Using MATLAB Neural Network Toolbox, a feed-forward ANN model was designed using back-propagation training algorithm. For each series of adsorption data, upper and lower temperature were used as the training data set to fit the temperature dependent neural network isotherm and the remaining

series (intermediate temperature) was used as the validation data set to assess the performance of the neural network predictions for the isotherm data that were not used during the fitting process. As can be seen from Figs. 2–6, the neural network model is able to predict very well the observed data points for both the training and validation data sets.

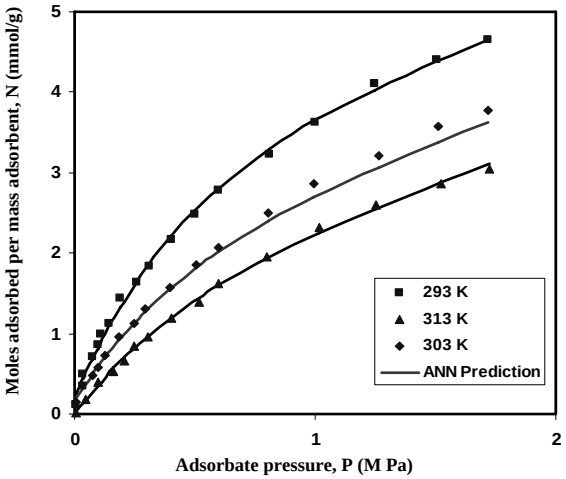

Figure 3. Comparison of the experimental adsorption data for CH_4/activated Carbon measured by Buss[13] with ANN(solid line)

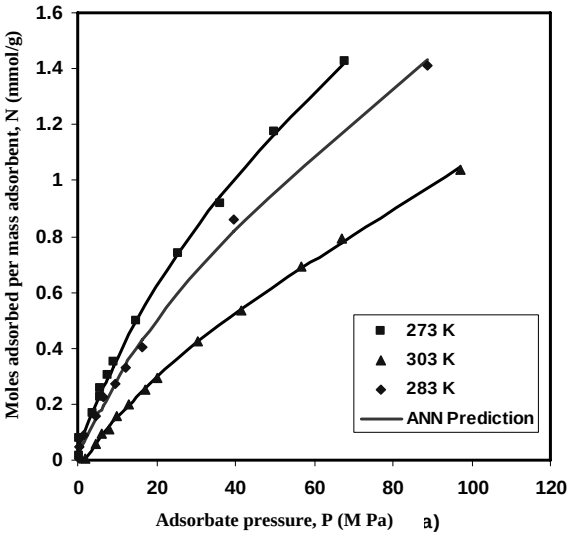

Figure 4. Comparison of the experimental adsorption data for CH_4/Ajax Activated Carbon measured by Qiao an Hu[12] with ANN(solid line)

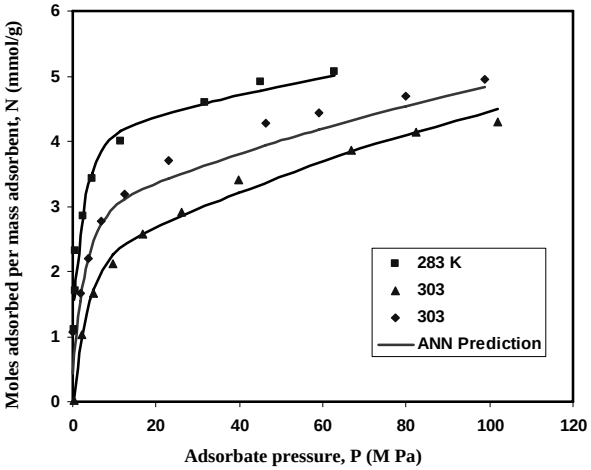

Figure 5. Comparison of the experimental adsorption data for C_3H_8/Ajax Activated Carbon measured by Qiao an Hu[12] with ANN(solid line)

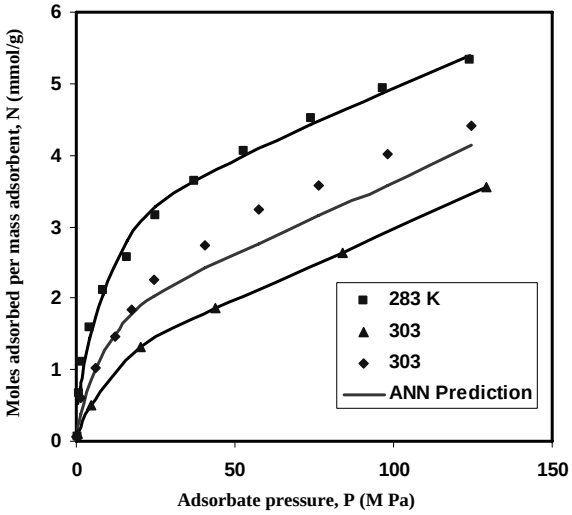

Figure 6. Comparison of the experimental adsorption data for C_2H_6/Ajax Activated Carbon measured by Qiao an Hu[12] with ANN(solid line)

4. Conclusions

In this study, the ability of neural networks was examined for their effectiveness to represent a wide array of adsorption data for the case of energetically heterogeneous solid surfaces. The model proved adept at fitting isotherms of adsorbate-adsorbent systems over a wide range of temperature. So it can be concluded that the application of ANN

models may be considered as an alternative for description of behavior of adsorption data for the case of energetically heterogeneous solid surfaces.

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