Separation Science and Technology
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713708471

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To cite this Article Yang, M. , Hubble, J. , Lockett, A. D. and Rathbone, R. R.(1996) 'A Neural Network Model for Prediction of Binary Adsorption Using Single Solute and Limited Binary Solute Adsorption Data', Separation Science and Technology, 31: 9, 1259 — 1265
To link to this Article: DOI: 10.1080/01496399608006949
URL: http://dx.doi.org/10.1080/01496399608006949

SEPARATION SCIENCE AND TECHNOLOGY, 31(9), pp. 1259–1265, 1996

A Neural Network Model for Prediction of Binary Adsorption Using Single Solute and Limited Binary Solute Adsorption Data

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ABSTRACT

A simple neural network model was used to predict binary solute adsorption onto granular activated carbon (GAC). While some data on binary adsorption were required, the neural network could be effectively trained using predominately single solute adsorption data, and only a limited number of data sets (<10) were necessary for effective performance. Once trained, the network was capable of predicting binary solute adsorptions even for systems showing nonideality.

Key Words. GAC; Multisolute adsorption; Neural network

INTRODUCTION

Adsorption of organic pollutants onto activated carbon has proved to be an economical and efficient method for the treatment of both drinking and wastewater. In most practical cases a number of pollutant molecules will be present, and competitive adsorption, which may have significant influences on the adsorption performance, is likely. Hence, reliable data on multisolute adsorption systems are essential for effective adsorptive based process design, scale-up, and optimization. A number of authors

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have addressed the measurement of multisolute adsorption isotherms (1, 2). However, as such measurements are extremely tedious and time consuming, prediction of multicomponent adsorption behavior has attracted increasing attention. Yen and Singer (3) employed the ideal adsorbed solution method to predict the adsorption from a mixture containing phenol and substituted phenols, and Annesini et al. (2) used the same method for adsorption of some other organic compounds onto granulated activated carbon (GAC). Although successful for a number of binary solute systems, this method failed to give a satisfactory prediction for systems which showed significant deviation from the assumptions of the model (2). This suggests that a more generic solution requires a different approach. Given that an intrinsic relationship will exist between single and multisolute systems in terms of their adsorption behavior, this relationship, though possibly complex, should be identifiable using an artificial neural network (ANN) approach (4), employing a training protocol based on a limited range of experimental values.

This note reports results which suggest that a neural network is an effective tool for prediction of multisolute adsorption. Experimental data reported by Annesini et al. (2), and our own experimental results on phenol and the herbicide 4-chloro-2-methyphenoacetic acid (MCPA), were used for the neural network training and testing. Experimental data on the binary adsorption of methoxyphenol (MP)/*o*-cresol reported by Martin and Al-Bahrani (5), which were not included in the training sets, were also used to assess the effectiveness of the network's predictive capability.

TRAINING SAMPLE SERIES, NETWORK INPUT CONFIGURATION, AND NETWORK TRAINING

The neural network used in this work, shown in Fig. 1, was similar to that reported previously (6, 7). The training sample series consisted of six single solute adsorption data sets representing the adsorption systems GAC with acetone, propionaldehyde (PA), methyl isobutyl ketone (MIK), sucrose, phenol, and MCPA, and 3 binary-adsorption data sets representing the binary systems GAC with acetone/MIK, acetone/PA, and acetone/sucrose. The first four single solute data sets and the three binary system data sets were taken from Annesini et al. (2) by either picking the reported experimental points or by calculation using their reported Langmuir parameters. The network input consisted of five elements as shown in Fig. 1. These are constructed as follows:

x1 Liquid phase concentration (mmol/L) used to determine the adsorption isotherms of components 1 and 2.

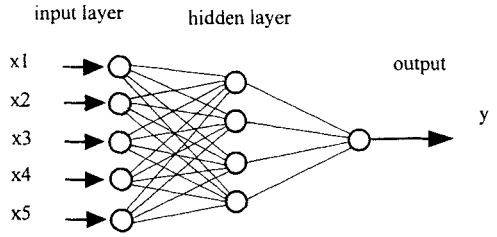

FIG. 1 Neural network structure.

x2 Adsorbed concentration (mmol/g) for solute 1 as a single component, determined at the liquid phase concentrations given in x1.

x3 Adsorbed concentration (mmol/g) for solute 2 as a single component, determined at the liquid phase concentration given in x1.

x4 The concentration of solute 1 (mmol/L) in the binary system scaled by its Langmuir dissociation constant, i.e., C_1/K (value set to zero for a single solute system).

x5 The adsorbed concentration of solute 1 (mmol/g) which could result from the liquid phase concentration used in x4 if competition from solute 2 is ignored (value set to zero for a single component system).

The network training target, Y, is the adsorbed concentration of component 2, corresponding to the liquid phase concentration specified in input x1 in the presence of component 1 at the concentration specified in input x4. Hence, once trained, the ANN should be capable of predicting the adsorption isotherm of one compound in the presence of any given concentration of the other.

The network training was carried out using a commercial neural network package (Neudesk2, 1993) on a 486 IBM compatible computer. Both standard backpropagation and stochastic backpropagation training methods were attempted. In this case the training performance was more effective using the stochastic backpropagation method, taking only a few minutes to reach the stage where the average error between the network output and the given target was reduced to 1.1%.

RESULTS AND DISCUSSION

Having achieved convergence in the training stage, the neural network was tested with binary adsorption data which did not form part of the

training sample series. Figures 2–5 show the network correlation for the system acetone/MIK, and predictions for MIK/sucrose, MP/*o*-cresol, and phenol/MCPA, respectively. The correlation for acetone/MIK and predictions for MIK/sucrose and phenol/MCPA are in good agreement with experimental results, while the prediction for MP/*o*-cresol is reasonable. It is worth noting that no binary data for MIK/sucrose, and phenol/MCPA, and no data at all for MP/*o*-cresol were involved in the training sets, therefore in these cases the network proved capable of recognizing the competitive effect of binary adsorption. Annesini et al. (2) found that the prediction of binary adsorption by means of an ideal adsorbed solution model was not fully satisfactory for systems containing sucrose, which was thought to be due to the nonideality of the adsorbed phase. Using their approach, the activity coefficients of the adsorbed phase were introduced to account for this nonideality, so that a better agreement between the calculated and experimental values could be obtained. However, as these activity coefficients must be obtained by fitting binary adsorption experimental data, the predictive potential of the method is significantly reduced. In contrast, the neural network model was able to quantify this nonideality through a learning program, and to give satisfactory predictions for such systems.

It was found that the most difficult step in this neural network application was the identification of the critical components of the input data to allow construction of training sample series which captured the essential

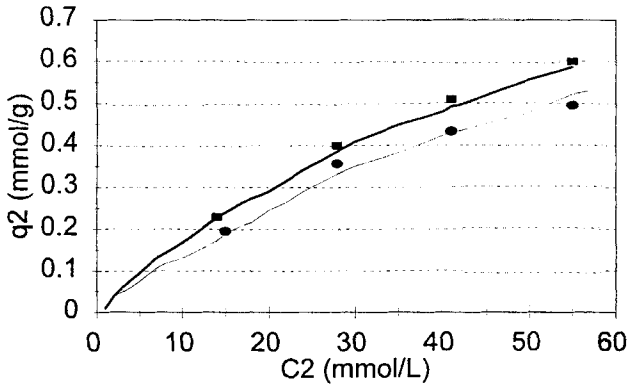

FIG. 2 Network correlation of adsorption isotherm of bisolute system: MIK (1)/acetone (2). Initial concentration of MIK in liquid phase: (■) C_1 = 5.1 mmol/L; (●) C_1 = 9.5 mmol/L. Lines: Network correlated isotherms.

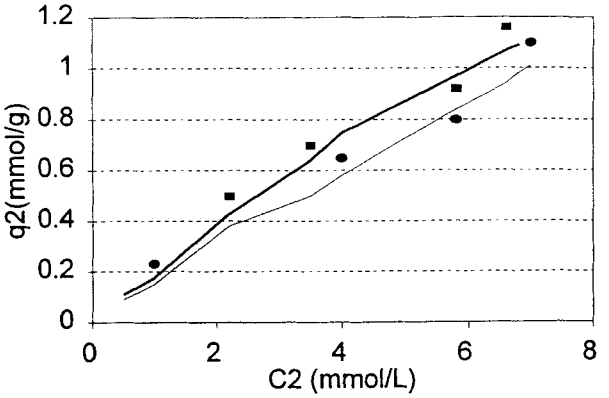

FIG. 3 Network prediction of adsorption isotherm of bisolute system: Sucrose (1)/MIK (2). Initial concentration of sucrose in liquid phase: (■) C_1 = 10 mmol/L; (●) C_1 = 20 mmol/L. Lines: Network predictions.

features of the system. This is a common problem with ANNs and has been noted by other authors (8).

Use of Langmuir parameters instead of real data on single solute adsorption, represented by x2 and x3, to form the network input was attempted, but this resulted in poor training fits. Initially, data of binary adsorption containing sucrose were not included in the training, and while the net-

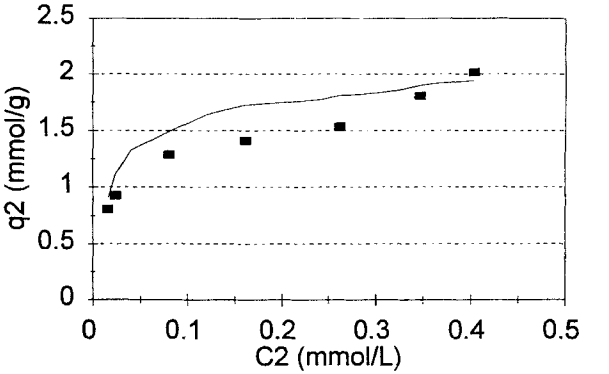

FIG. 4 Network prediction of adsorption isotherm of bisolute system: *o*-Cresol (1)/MP (2). Initial concentration of *o*-cresol: q_1 = 1 mmol/g in solid phase, and C_1 = 0.1 mmol/L (estimated). Line: Network prediction.

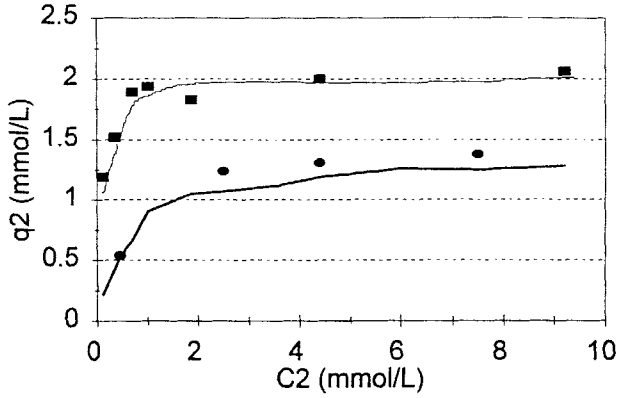

FIG. 5 Network prediction of adsorption isotherm of bisolute system: MCPA (1)/phenol (2). Initial concentration of MCPA in liquid phase: (■) $C_1 = 0$; (●) $C_1 = 0.08$ mmol/L. Lines: Network predictions.

work gave perfect training fits, its predictions were poor for systems containing sucrose. This suggested that some essential features of the systems containing sucrose were missing in the training, and these features might represent nonideality. To overcome this deficiency, the training sample series was reconstructed to include data for sucrose. Essentially, it appears that if the network has learned patterns A–B and A–C, it is able to predict pattern B–C. While such a network might be capable of giving a reasonable prediction for a totally new pattern, this is not guaranteed, and more system specific training sets may be needed. In principle, it should be possible to represent a range of highly complex relationships by using a complex network structure and a wide range of training sets. However, in practice a more limited approach based on the components known to be present in the system is likely to be sufficient and certainly will lead to significantly reduced training overheads. Although currently evaluated for binary systems, an extension to include ternary and quaternary systems should be possible in principle and will be the aim of further study.

SUMMARY

A neural network model has been shown to be effective for the prediction of binary adsorption isotherms provided it is trained with a suitable range of input data. The network model can effectively recognise nonideality, and remains predictive for nonideal systems. Unlike traditional em-

pirical or semiempirical models which require tedious experimental work to obtain a large number of data on multicomponent adsorptions, the neural network model requires very limited multicomponent data.

ACKNOWLEDGMENT

The authors would like to thank the SERC for financial support under Grant GR/J15292.

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Received by editor August 7, 1995