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DESIGNING AND ANALYZING FIXED-BED ADSORPTION SYSTEMS WITH ARTIFICIAL NEURAL NETWORKS

IMAD A. BASHEER

YACOUB M. NAJJAR

Kansas State University, Manhattan

ABSTRACT

Adsorption in fixed beds is a common unit process in water treatment and in a large number of separation technologies. The dynamics of fixed-bed adsorption are commonly described by mathematical models which require a thorough understanding of the complex phenomena. The mathematical models of adsorption, which are a set of partial differential equations describing mass balances and transfer, usually require numerical solution. This article describes the application of artificial neural networks to the problem of predicting the breakthrough time, a critical parameter in adsorption in fixed beds. The approach employed also can be used to develop more general predictive neural networks that deal with a large number of situations encountered in fixed-bed adsorption. The ability of the developed neural network to predict the breakthrough time is found to be comparable to that for a mathematically-based model. The advantages of the neural networks over the conventional mathematical models as well as their limitations are stated.

INTRODUCTION

For most applications in water purification, material recovery, and separation technology, adsorption has historically been regarded as an effective practice. In the drinking water industry, activated carbon, as an adsorbent, has been widely used for many applications. Typically, the contaminated water is contacted with activated carbon in a large-scale contacting system. The most common type of contactor in water and wastewater treatment applications is the fixed-bed reactor, where the adsorbent is held stationary in a column during the operation, and the

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water to be treated is passed continuously through the column, where adsorption of the contaminant occurs. Adsorption initially takes place on the adsorbent close to the inlet of the column and proceeds to the exit as the uppermost fractions of the bed become saturated. This gives rise to a concentration front that travels along the bed as time progresses. Therefore, the effluent concentration could vary from zero at the initial stages of operation to the maximum value (influent concentration) at a later stage when the entire bed gets fully saturated with the contaminant. The variation of the effluent concentration with time is usually described by a breakthrough curve, as shown in Figure 1. This type of curve summarizes the effects of both the rate and the equilibrium processes of adsorption. Along the course of adsorption process, the effluent concentration passes through some point where the objective (water quality) is no longer met. As shown in Figure 1, this point is called the breakthrough point which indicates the time for termination of the operation and signifies the required subsequent replacement or generation of the contaminated adsorbent. In drinking water applications, the effluent water is

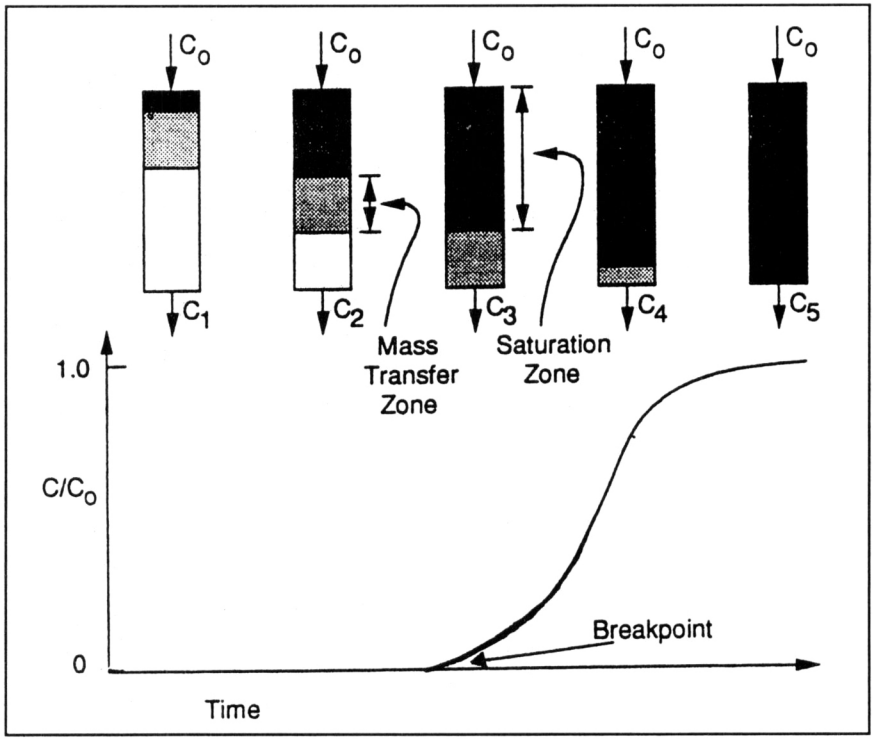

Figure 1. Schematic of a representative breakthrough curves of a fixed-bed adsorber.

allowed to have a very small value of contaminant concentration that represents the maximum contaminant level (MCL) value as needed by the end user. Therefore, the breakthrough point is a critical parameter in the operation and design of adsorption systems. The time at which the breakthrough point occurs is called the the breakthrough time which indicates the time the column should be taken out of service. Models that predict the breakthrough curves of fixed-bed adsorbers are mathematically-based models that require a good understanding of the physical phenomenon. Such models are difficult to formulate and usually are solved numerically using finite element or finite difference methods. Moreover, employing these mathematically-based models requires long and expensive computer running times which might render these models impractical. In contrast to these detailed procedures of developing the model and their solution procedures, the rapidly evolving potential of artificial neural networks to predict the breakthrough time is studied in this article. For the sake of completeness and clarity, models of prediction in fixed-bed adsorption that are typically used in the area of water and wastewater treatments are briefly discussed next, and the concept of neural networks, and the areas in civil engineering where they have been applied, are also reviewed.

FACTORS AFFECTING ADSORPTION IN FIXED BED

A key element in the design of fixed-bed adsorbers for water purification, the breakthrough time is influenced by a wide variety of parameters pertaining to physical and chemical characteristics of both the contaminant and the adsorbent, as well as to the other operating and hydrodynamic conditions. The influence of adsorption by the adsorbent is reflected in its dependence on the adsorption equilibrium isotherm and the particle size distribution of the adsorbent. The adsorption isotherm refers to the equilibrium attained between the adsorbate and the adsorbent at constant temperature. This might be embodied in any of several forms of relationships, depending on the kind of interaction between the adsorbate and the adsorbent [1]. In fixed-bed adsorption, bed dimensions also have an effect through their influence on the speed by which the concentration front travels along the bed. For two similar adsorbents, the finer the particles, the greater the utilization of the adsorbent, and the higher the adsorption. Other parameters are shown in Table 1 which also summarizes the effect of *increasing* the magnitude of each parameter (while keeping the others at their constant values) on the breakthrough time.

MATHEMATICAL MODELING OF FIXED-BED ADSORPTION

Many investigators have extensively pursued the development of various mathematical models that describe the kinetics of the adsorption process and the

Table 1. Effect of Increasing the Value of Each Parameter on the Breakthrough Time

Parameter	Symbol	Breakthrough Time (Tb)
Influent concentration	C_0	Decreases
Influent flowrate	Q	Decreases
Cross-sectional area	A	Increases
Weight of adsorbent	W	Increases
Length of adsorbent bed	P	Increases
Solution temperature	T	Generally decreases
Solution pH	pH	Variable
Bed voidage	ε_b	Decreases
Particle diameter	d_p	Increases
Intraparticle porosity	ε_p	Increases
External mass transfer coefficient	K_f	Increases
Surface diffusion coefficient	D_s	Increases
Isotherm expression	q = f(C)	Increases

dynamic behavior of fixed-bed adsorbers (e.g., [2-4]). In most of these models, adsorption is assumed to proceed in a combination of three processes: mass transfer of adsorbate from the bulk liquid to the particle surface, intraparticle transport within the particle, and adsorption of the adsorbate onto the adsorbent (this is a very fast step and is usually ignored in modeling). Figure 2 shows schematically the three mechanisms involved in the adsorption process. All mathematically-based models are capable of predicting the breakthrough curve from a set of known parameters pertaining to adsorbate, adsorbent, and hydrodynamic conditions. Generally, a fixed-bed adsorption model is simply a set of partial differential equations that describe the mass balance of adsorbate in both the entire bed and the adsorbent particle, linked to an adsorption equilibrium expression. Depending on the assumption and simplifications involved in developing the model and the type of the initial and boundary conditions imposed, the model in most cases may not have an analytical solution, and it is most likely that numerical techniques are needed for solution. The mathematical models, in principle, provide a method for design of fixed-bed adsorbers without conducting the extensive and lengthy type of laboratory- or pilot-scale experiments. The development of the partial differential equations that describe the mass balance in the bed and within the adsorbent particles will not be discussed in this article and the interested reader could be referred to Weber [5] and Ruthven [1] for additional knowledge. However, the HSDM model (Homogeneous Surface Diffusion Model) that has been used extensively, with success, in many areas of water treatment by activated

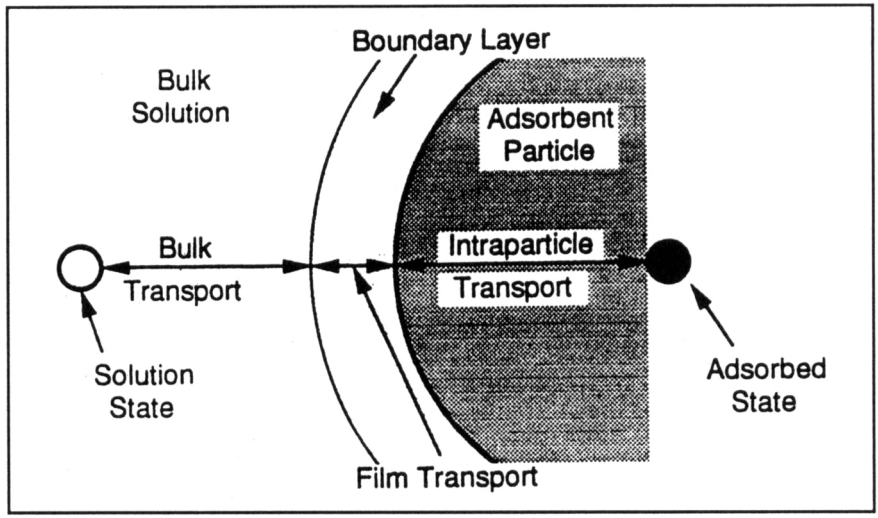

Figure 2. Mass transfer steps in adsorption onto porous adsorbent.

carbon [6-8] will be presented herein, as it represents the main tool for constructing the present adsorption database.

The Fixed-Bed Adsorber Model HSDM

The rate of accumulation of adsorbate on the surface of an adsorbent particle can be described by the following partial differential equation and initial and boundary conditions [6]:

$$\frac{\partial q}{\partial t} = \frac{D_s}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial q}{\partial r}\right)$$

$$@t = 0;\ o \le r \le R_p:\ q = 0$$

$$@t \ge 0;\ r = 0:\ \frac{\partial q}{\partial r} = 0 \qquad (1)$$

$$@t \ge 0;\ r = R_p:\ R_p{}^2 k_f (C - C_s)/\rho = \frac{\partial}{\partial t}\int_0^{R_p} q r^2 dr$$

$$@r = R_p; C_s = f(q_s)$$

The mass balance of the adsorbate in the entire bed and the corresponding initial and boundary conditions may be written as:

$$\frac{\partial C}{\partial t} = \left[-v \frac{\partial C}{\partial z} - \frac{3(1-\varepsilon_b)}{R_p \varepsilon_b} \right] k_f (C - C_s)$$

$$@t = 0;\ 0 \le z \le L:\ C = 0 \tag{2}$$

$$@t \ge 0;\ z = 0:\ C - C_o$$

where r is the radial distance within the spherical adsorbent particle, R_p is the radius of the particle, z is the axial distance along the column, L is the length of the column, v is the superstitial fluid velocity in the bed, ε_b is the bed porosity, q is the surface adsorbate concentration, D_s is the solid phase diffusion coefficient, C is the concentration of adsorbate in the liquid phase, C_0 is the influent concentration, C_s and q_s are the adsorbate liquid and solid concentration at the external surface of the particle, respectively, ρ is the apparent density of the particle, k_f is the mass transfer coefficient, and t is time since the beginning of operation. The equation $C_s = f(q_s)$ represents the adsorption equilibrium isotherm. The present model equations are solved numerically by Thacker et al. [9], for single and bisolute cases with uniform adsorbent size, using the orthogonal collocation method. This method is used to convert the partial differential equations into first order ordinary differential equations which are then solved using the integration routine GEAR. It is to be mentioned herein that the solid phase diffusion coefficient D_s has to be determined from batch experiments. On the other hand, the mass transfer coefficient k_f also can be determined from batch experiments as well as from correlations such as those described by Dwiwedi and Upadhyay [10]. The present model is used in this research to create the fixed-bed adsorption database.

APPLICATIONS OF NEURAL NETWORKS

Artificial neural networks have recently attracted the interest of many investigators in several fields in civil engineering. Such applications encompasses topics in the transportation engineering area [11, 12], construction simulation and cost analysis [13, 14]; seismic hazard prediction [15], river flow prediction [16], simulation of structural analysis [17], structural optimum design [18], characterization of stress-strain material behavior [19], contaminated aquifer remediation [20], and perdition of compacted clay permeability [21].

Neural network development is inspired by studies conducted on the brain and nervous systems in biological organisms and by the advances encountered in the computer technology. Neural networks are constructed from a number of parallel operating processors, called neurons, in a highly interconnected network. The architecture of a simple neural network consists of an input layer containing the input nodes, an intermediate layer called the hidden layer which accommodates the hidden nodes, and the output layer which contains the output elements. A basic

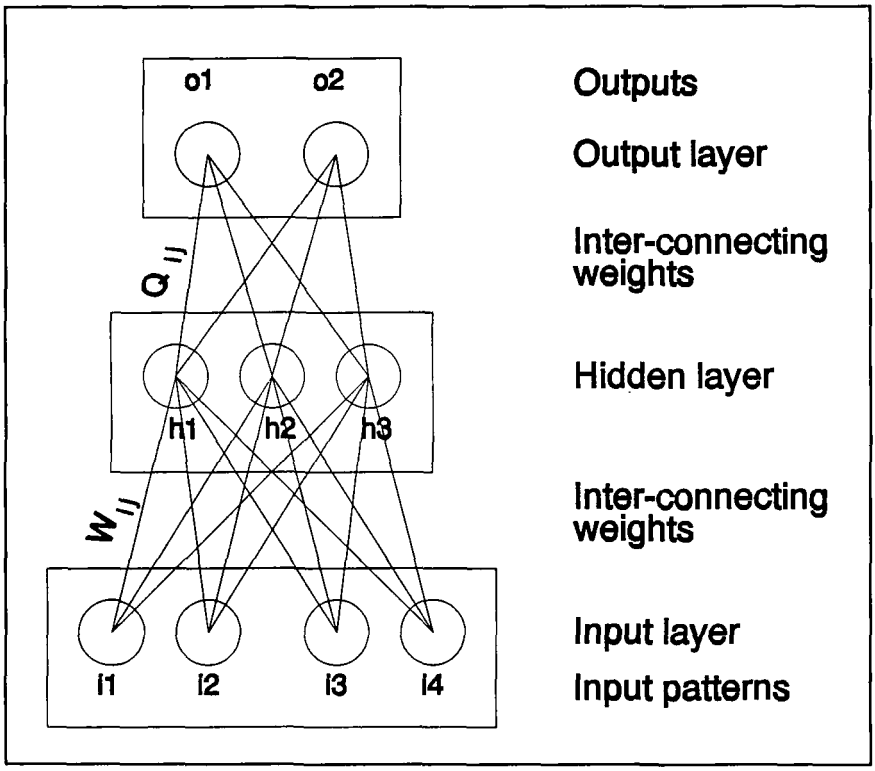

Figure 3. Basic anatomy of a multi-layered neural network.

anatomy of a three layer representative network is shown in Figure 3. Neural networks can analyze and process a large number of input data to establish patterns for a situation where the relationships between the inputs and the outputs are not known due to complexity of the problem or unavailability of an expert. A neural network can be trained by the aid of a supervised learning algorithm, using back propagation error correction to adjust the weights associated with each node. For additional understanding of the different learning procedures and the mechanisms and architecture of neural networks, the reader could benefit from the available literature such as [19, 22-25].

In the present research, the most popular type of networks, the backpropagation network, is employed to model the breakthrough time for adsorption in fixed-bed adsorbers. This type of network and algorithm was chosen because of its observed success in modeling complicated phenomena in civil engineering applications. The algorithm for the back propagation learning is discussed in the following section.

THE BACK PROPAGATION LEARNING ALGORITHM

Associated with each connection is a numerical value representing the strength or the weight of that connection (example: W_{ij} = strength of connection between an input unit i and a hidden unit j). The connection strengths are developed during the training of the neural network. At the beginning of the training process, the connection strengths are assigned random values. As inputs and outputs are presented during the training, the adopted rule of learning modifies the connection strength in an iterative process. When the iterative process has converged, the weights learned are then stored for later use of the network to evaluate new sets of inputs when presented. After the weights are learned, analysis of new patterns only takes few seconds. A step-by-step summary of the back-propagation learning algorithm adopted in this study is presented herein:

1. Initialize weights and thresholds (biases): Set all connecting weights between input units and hidden units (W_{ij}), hidden units and output units (Q_{ij}), thresholds of hidden units (θ_i) and threshold of output units (ϕ_i) to random values in the range of [+1, –1].

2. Present input and target: Present an input vector representing each pattern to be learned and the target.

3. Propagate the simulation of the inputs: Compute net input, N_i, to hidden units by weighing and integrating the outputs (o_i) impinging on the units.

$$N_i = \sum_j W_{ij} O_j \tag{3}$$

Compute the output of the nodes using a differentiable sigmoid nonlinear activation function

$$O_i = \frac{1}{1 + e^{-(N_i + \theta_i)}} \tag{4}$$

For output units, follow the same procedure as for hidden nodes.

4. Back-propagate errors: Start at output units and work back to hidden units. During this backward pass, compute an error signal δ_i for each of the output unit. In this case, δ_i is determined by

$$\delta_i = (t_i - o_i)\, o_i\, (1 - o_i) \tag{5}$$

where o_i is the activation of the output unit i and t_i is the desired output of the i^{th} unit. The error signal is then back-propagated to each hidden unit connecting with the output unit. The error signal for each hidden unit is determined by

$$\Delta_i = o_i\, (1 - o_i) \sum_k \delta_k Q_{ki} \tag{6}$$

where Q_{ik} is the connecting weight from hidden unit i to output unit k. The summation term means that the influence of the error signals from all output units is accumulated.

5. Adjust weights: The weight (W_{ij} or Q_{ij}) on each connecting line at training step number n is adjusted according to the following training rules

$$Q_{ij(n+1)} = Q_{ij(n)} + \beta\delta_i o_j + \alpha\,(Q_{ij(n)} - Q_{ij(n-1)}) \tag{7}$$

$$W_{ij(n+1)} = W_{ij(n)} + \beta\Delta_i o_j + \alpha(W_{ij(n)} - W_{ij(n-1)}) \tag{8}$$

in which β denotes the training coefficient and α represents the momentum coefficient. To ensure that the learning process is incremental, β should be in the range of [0, 1], while the recommended value of α should be in the range of [0.075, 0.9].

6. Adjust thresholds: Internal unit (hidden and output) thresholds are adjusted in a similar manner by assuming that they are weights to a unit from a unit whose activation is always 1.0. Therefore, the thresholds are adjusted as follows

$$\varphi_{j(n+1)} = \varphi_{j(n)} + \beta\delta_j \tag{9}$$

$$\theta_{j(n+1)} = \theta_{j(n)} + \beta\Delta_j \tag{10}$$

7. Repeat steps 2 to 6 whenever a new pattern is presented.

GENERATION OF THE FIXED-BED ADSORPTION DATABASE

In order to develop a neural network, the input data must be sufficiently abundant and must cover a relatively wide range of the domain to insure the capability of the network to capture all features and subfeatures embodied in the phenomenon to be explored. Therefore, the database is an important and critical element in developing a sufficiently accurate predictive network. In this section, the database, representing input and output data, for fixed-bed adsorption is constructed. The success of the neural network to capture all details associated with a certain engineering phenomenon lies mainly in the size and credibility of the data the network is presented with. In the breakthrough curves of the fixed-bed adsorbers, the input variables are assumed to be those listed in Table 1. The database should then be built from combination of these input data and from the breakthrough time that represents the single output. The breakthrough time is usually extracted from results of experiments conducted on laboratory or pilot-scale adsorption columns. Because of the lack of a sufficient number of cases on fixed-bed adsorption that could form a database of reasonable size, the mathematical model (HSDM) presented earlier is used to generate the database for a large number of cases by varying the input data. This technique has the merit that the

HSDM was previously found to be able to predict, with a relatively high degree of accuracy, the breakthrough curves of organic compound adsorption onto the granular activated carbon [6, 7, 9, 26, 27]. Therefore, the available mathematical model could reasonably replace the lengthy and extensive type of fixed-bed adsorption experiments. It is the objective of this article to check the ability of a simple neural network to simulate the accuracy of the computationally expensive HSDM adsorption model. The simple neural network would significantly reduce the computer time required to solve the complex fixed-bed adsorption design problem.

Development of the Problem Domain

The HSDM computer program requires several input variables (also are shown in Table 1). The problem formulated in this research involves phenol adsorption from water on granular activated carbon (GAC). The following assumptions and data are used in running the HSDM model program:

(i) the solid phase diffusion coefficient, D_s, of phenol adsorption on activated carbon is assumed to be constant regardless of the adsorbent particle size. A value of $D_s = 3.5 \times 10^{-8}$ cm/sec [6] is assumed to be representative for all runs,
(ii) an apparent density of carbon of 0.68,
(iii) the three-parameter isotherm expression $q = AC/(1+BC^{\beta})$, where A, B, and β are constants is used to run the program. For phenol adsorption, onto GAC, from aqueous solution at temperature of 25°C and a pH of 7, the values of A, B, and β are taken as 15.11, 7.547, and 0.8685, respectively [6],
(iv) a constant bed porosity (bed voidage) of 0.40 is assumed regardless of the adsorbent particle size. This is not a very harsh assumption, as the particle sizes, that are usually encountered in GAC application, might vary within a narrow range, and
(v) uniform adsorbent particle size, constant influent flowrate, and constant influent concentration of phenol.

With these assumptions and input data, seven input variables are found necessary to run the program. These are: the influent concentration, C_0, the influent flowrate, Q, the weight of GAC in the bed, W, the diameter of the cylindrical adsorber, D, the length of the bed, L, the adsorbent particle diameter, d_p, and the external mass transfer coefficient, k_f. However, the length of the bed could be related to both weight of GAC and the adsorber diameter. Moreover, the external mass transfer coefficient could also be related to the cross sectional area of the adsorber, the flowrate, and the particle diameter, using the correlation of Dwiwedi and Upadhyay [10]. For this problem, the length of the adsorber in (cm) is calculated from [L = 2.45 W/A] where A is the cross sectional area of column in

cm^2, and W in grams (g). Using the correlation of Dwiwedi and Upadhyay [10], the external mass transfer coefficient, k_f (in cm/sec), is derived as [$k_f = 9.7 \times 10^{-4}$ d_p–0.72 $(Q/A)^{0.28}$], where Q is expressed in cm^3/sec, d_p in cm, and A in cm^2. Therefore, the independent parameters for the fixed-bed adsorption process are only five: Co, Q, A, W, and d_p. These input variables are shown schematically on a representative column adsorber in Figure 4.

To generate the database, several values of the various parameters are assigned and the program is run to obtain the predicted breakthrough curves. The data of the different runs are designed such that they simulate only laboratory fixed-bed adsorption experiments. To reduce the number of trials (runs), both Q and A were fixed [Q = 500 cm^3/sec. and A = 20.27 cm^2 (i.e. D = 2")]. Therefore, all runs correspond to a single column treating phenol laden water flowing at a uniform flowrate. The input variables are consequently reduced to three: C_0, W, and d_p. The present problem is a frequently encountered optimization design problem in

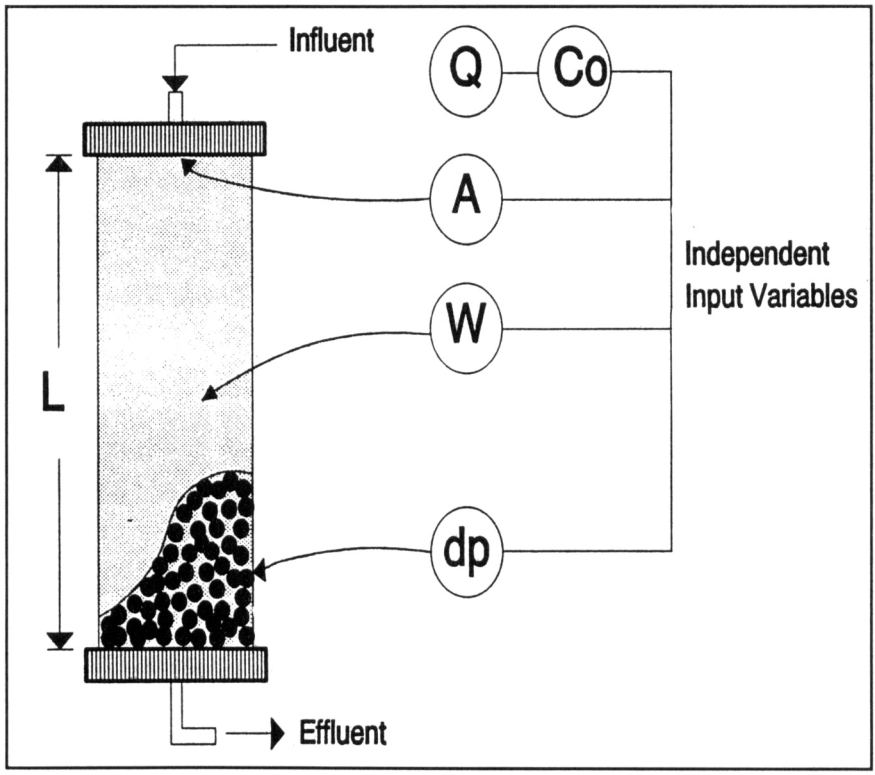

Figure 4. Schematic of a fixed-bed adsorber showing the independent input variables.

the field of water and wastewater treatment by adsorption. The values tested for these three input variables are summarized in Table 2. It is worthy to mention herein that the three particle sizes; represented by their geometric mean particle radii (R_p = 0.077, 0.055, and 0.027 cm) correspond to the U.S. mesh sizes (retained/passing): #12/#14, #16/#18, and #30/#35, respectively). The output of each run is simply the concentration of phenol in the effluent as function of time. The breakpoint is assumed to occur whenever the effluent concentration reaches 5

Table 2. The Sets Used in Training the Neural Network

Set #	Co (mg/L)	W (g)	Rp (cm)	Tb (min)
1	50	100	0.077	137.7
2	600	100	0.077	7.2
3	1000	100	0.077	3.3
4	50	400	0.077	1705.7
5	200	400	0.077	491.1
6	600	400	0.077	129.2
7	1000	400	0.077	63.2
8	50	1000	0.077	5077.0
9	200	1000	0.077	1652.3
10	600	1000	0.077	545.7
11	1000	1000	0.077	296.3
12	50	100	0.055	289.6
13	200	100	0.055	73.5
14	600	100	0.055	16.8
15	1000	100	0.055	7.9
16	200	400	0.055	624.2
17	600	400	0.055	196.0
18	1000	400	0.055	103.0
19	50	1000	0.055	5345.9
20	200	1000	0.055	1784.5
21	1000	1000	0.055	388.3
22	50	100	0.027	484.6
23	200	100	0.027	155.7
24	600	100	0.027	49.3
25	1000	100	0.027	26.1
26	50	400	0.027	2173.3
27	200	400	0.027	737.8
28	600	400	0.027	282.0
29	1000	400	0.027	173.5
30	50	1000	0.027	5522.0
31	200	1000	0.027	1885.0
32	600	1000	0.027	747.0
33	1000	1000	0.027	477.0

Note: Co: Influent Concentration (mg/L); W: Weight of GAC in Bed (g); Rp: Radius of Adsorbent Particle (cm); Tb: Breakthrough Time (min).

percent of the influent concentration (i.e., $C_3 = 0.05\ C_0$). Some of the obtained breakthrough curves for various cases are displayed in Figure 5. These curves show the effect of influent concentration, particle size, and GAC weight on the breakthrough time. The breakthrough times for the different cases are summarized in Table 2, which also represents a collection of the training sets to be presented to the neural network for learning the embodied pattern.

DEVELOPING THE NEURAL NETWORK

In order to construct the fixed-bed adsorption neural network, the architecture has to be first identified. The supervised learning error backpropagation type of neural network is used in this work. This type of network was found to yield satisfactory generalizations in many applications. A computer program developed by the authors is used to train the neural network for the thirty-three training sets shown in Table 2. While the number of the input nodes in the input layer of the neural network is fixed at three and the output layer contains only the breakthrough time, the number of hidden nodes in the single hidden layer may vary. Hence, a trial-and-error procedure is used to determine the number of hidden nodes that yields the best generalization. This can be achieved by testing a trained network by applying several sets (or examples) that have never been presented to the network during its learning (i.e., the testing sets are not part of the training sets). Table 3 shows six sets that are used for testing the network. Also given in Table 3 are the exact values of the breakthrough time as determined by the computer program HSDM. A comparison of the different neural networks that vary by the number of hidden nodes can be seen in Table 4, which also shows the mean of absolute value of the relative error (MRE) between the exact (based on HSDM) and the predicted values for the training and the testing sets. As shown in Table 4, the network that yielded the lowest MRE is the one with ten hidden nodes. The ten-hidden-nodes layer network is shown in Figure 6 and can be used as a prediction tool for the breakthrough times for a given set of values. Moreover, this network can also be used as a tool to design the special case of fixed-bed adsorber system given in this article if the design life of the reactor is known (i.e., for a known breakthrough time). It is worth mentioning that the present network works with variables whose values fall within the ranges specified in Table 2. This network could, with an appreciable degree of accuracy, replace the HSDM mathematical model represented earlier by the numerical solutions to Eqs. 1 and 2. A comparison between the exact values and the corresponding values predicted by the ten-hidden nodes network for the six testing sets is shown in Figure 7. It is to be mentioned in this context that although the neural network developed in this article is of limited use, more general networks can be developed if the same procedure adopted herein is followed for more general cases. This can be implemented by increasing the number of input parameters to include other variables such as flowrate Q or adsorber diameter D.

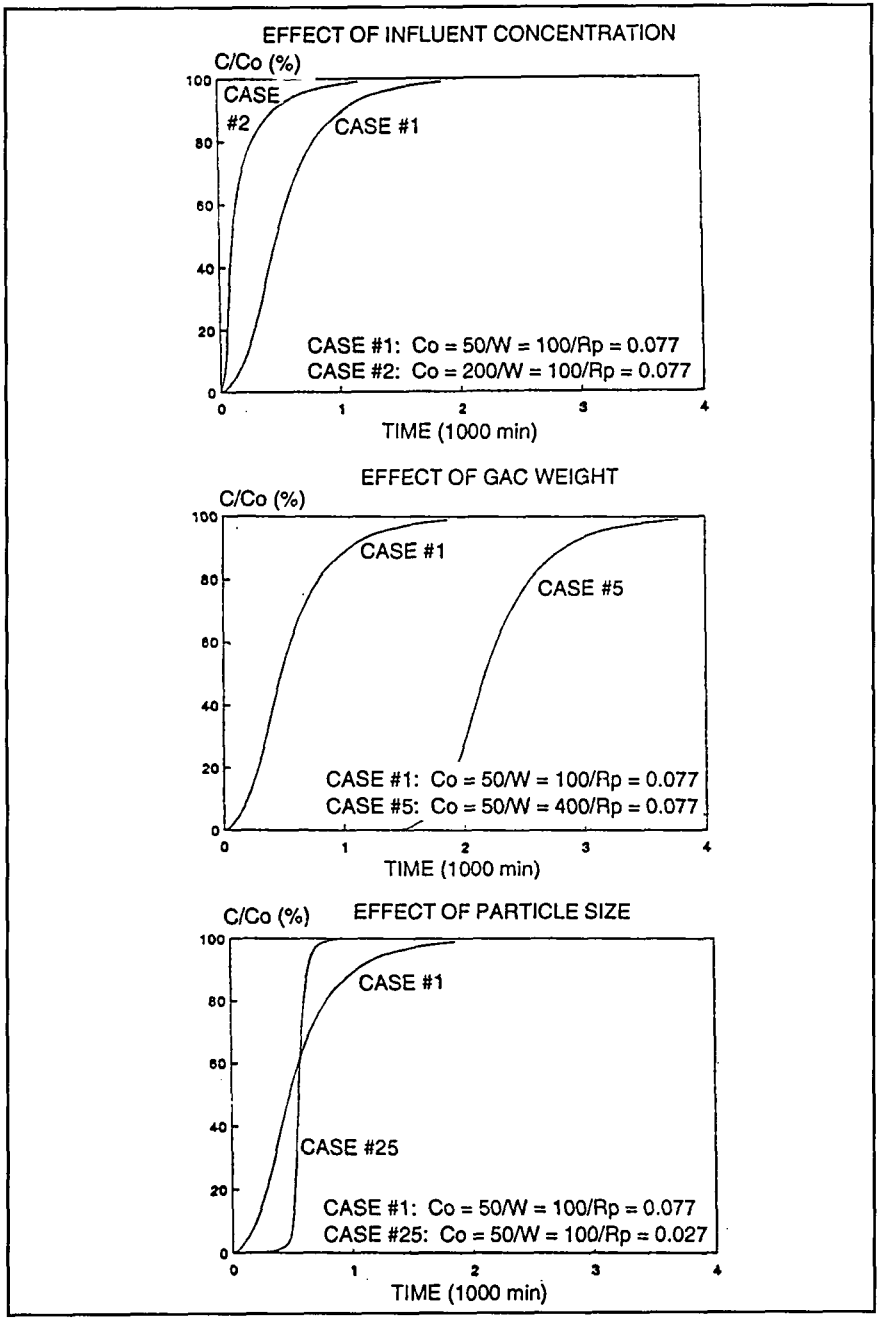

Figure 5. Breakthrough curves for some of the fixed-bed adsorber cases.

Table 3. The Sets Used in Testing the Neural Network

Set #	Co (mg/L)	W (g)	Rp (cm)	Tb (min)
1	200	100	0.077	32.9
2	500	400	0.055	1954.6
3	600	1000	0.055	656.3
4	400	600	0.065	479.9
5	700	500	0.0385	282.5
6	150	250	0.077	320.0

Note: Co: Influent Concentration (mg/L); W: Weight of GAC in Bed (g); Rp: Radius of Adsorbent Particle (cm); Tb: Breakthrough Time (min).

Table 4. Variation of the Mean Relative Error with the Number of Hidden Nodes

NH	Testing Sets MRE (%)	Training Sets MRE (%)
1	126.7	475.4
2	40.7	108.0
3	13.0	13.2
4	12.1	14.6
5	10.0	11.3
6	9.8	11.1
10	9.2	11.0
12	9.6	11.4
14	10.2	10.9

Note: NH: Number of Hidden Nodes; MRE: Mean of Absolute Values of Relative Error.

SENSITIVITY ANALYSIS OF THE INPUT PARAMETERS

In the developed design and prediction network, there are three input variables: input concentration, weight of GAC, and GAC particle radius. In order to determine the influence of each of these parameters on the predicted breakthrough time, sensitivity analysis is employed. This could be implemented by varying one parameter over certain range while keeping the other two at their fixed values and by observing the variation associated with the output. To avoid any bias in the case to be chosen for sensitivity analysis, an average representative case is derived by taking the averages of each of the input parameters for all cases shown in Table 2. The ten-hidden-nodes network, shown in Figure 6, is used to obtain the output

Connecting Weights for the Prediction Network with the 10 Hidden Nodes

Connecting Weights between Input Node, i, and Hidden Nodes, Wij			
Hidden Node, j	W1j	W2j	W3j
1	2.986	0.783	–0.18
2	–4.599	–0.999	–0.144
3	–1.297	–0.199	–1
4	–2.474	1.832	–1.341
5	–9.402	0.572	–0.944
6	–7.812	7.672	–1.381
7	–1.866	0.581	–1.732
8	–8.1	–0.416	0.893
9	–1.708	–0.279	–0.222
10	–16	3.898	–1.208

Thresholds of Hidden and Output Nodes

Hidden Nodes	Threshold Value
1	1.809
2	0.288
3	–0.566
4	0.833
5	–0.526
6	0.756
7	–0.853
8	–1.095
9	–1.974
10	–3.934
Output Node	
1	–2.539

Connecting Weights between Hidden Nodes, j, and Output Node, Qj1

Hidden Nodes	Qj1
1	–4.929
2	–1
3	–0.999
4	2.711
5	–0.248
6	4.374
7	–1.304
8	3.222
9	–0.168
10	11.528

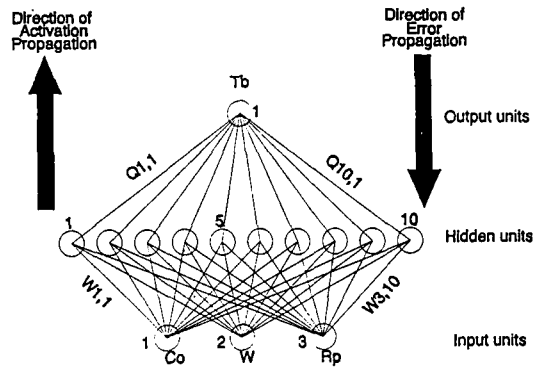

Figure 6. Architecture of the 10-hidden node prediction network and the connection weights.

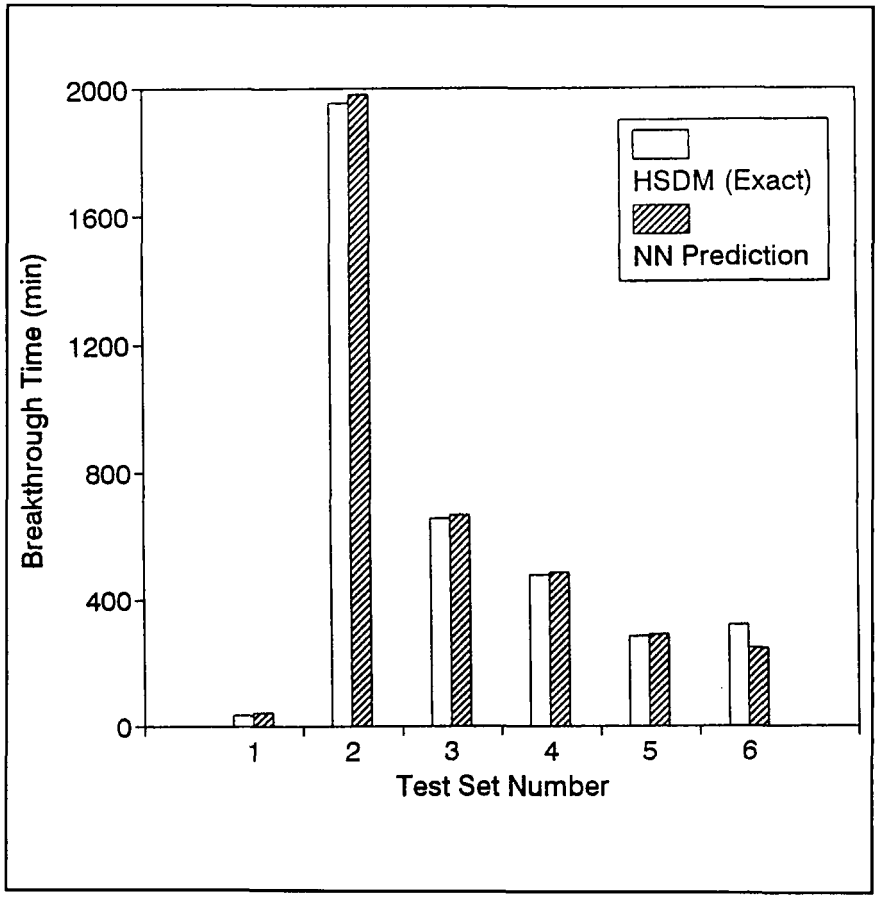

Figure 7. Comparison between exact (HSDM) and predicted (neural network) solutions.

breakthrough times. The average values for C_0, W, and R_p are calculated as 462.5 mg/L, 500 grams, and 0.053 cm, respectively. Using the ten-hidden nodes network, the breakthrough time for this *average case* was calculated as 337.4 min. To study the effect of perturbation associated with the three input parameters on the estimated breakthrough time, several runs using the ten-hidden nodes network are performed on the average case by varying the value of one of the input parameters through various percentages. It is important to notice that all perturbations are made within the ranges of the input parameters on which the neural network was developed. The results of sensitivity analysis obtained for the three input parameters (i.e., influent concentration, adsorbent weight, and particle radius) are shown in Figure 8. As shown in Figure 8, the sensitivity of the breakthrough time

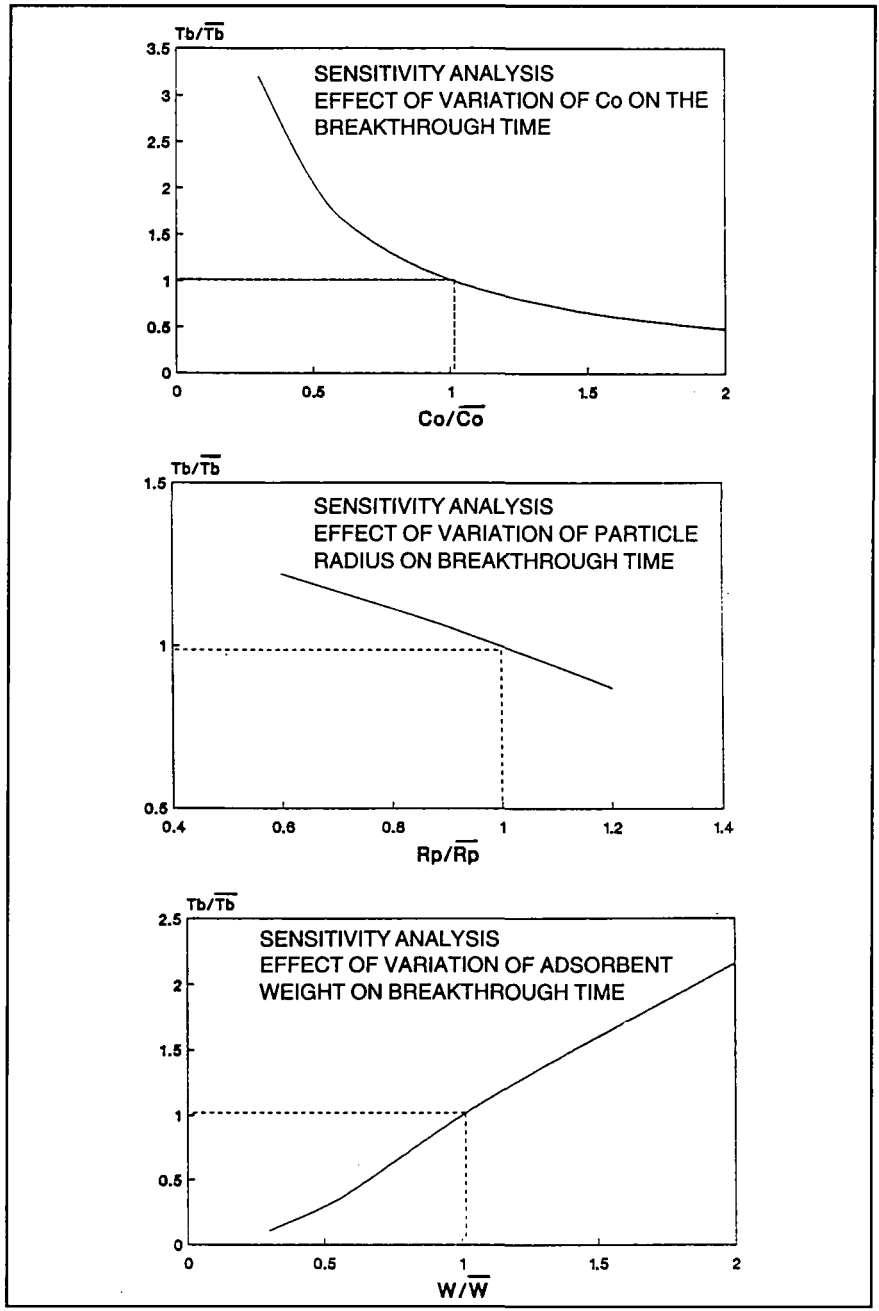

Figure 8. Results of sensitivity analysis of the three input parameters.

to the input parameters is given as a ratio from the average case values. The relative sensitivities for the three input parameters are also calculated from Figure 8 as the ratio between the normalized breakthrough time and the normalized parameter value (slope of the curve). A summary of the relative sensitivity parameters (as percentages) is shown in Table 5. As given in Table 5, for an influent concentration falling in the range 1.0-2.0 of the average C_o (i.e., 462.5-925.0 mg/L), the relative sensitivity is –52.0 percent. This value indicates that if the influent concentration increases by 10 percent, the effect on breakthrough time would be a decrease by 5.2 percent. As can be seen from Table 5, all parameters are relatively important and significantly influence the breakthrough time. This could be interpreted as showing the necessity of running the fixed-bed adsorption experiments under precise measurements of the three input parameters.

DISCUSSION AND CONCLUSION

In this article, although the example studied is quite specific, the same method of developing the database and the neural network can be employed to obtain a more generalized form of the prediction network. This can be implemented by incorporating the following modifications:

(i) the flowrate and the column diameter could be varied to generate a larger-size database. Including these parameters in the developed neural network would render the prediction network more nonspecific.

(ii) a larger number of adsorbates could also be tested and a more general neural network that is capable of dealing with several contaminants can be developed. To achieve this, a few more input nodes, representing the adsorption isotherm constants, can be added to the input layer. For the three-parameter isotherm $q = AC/(1+BC^{\beta})$, as an example, the three additional input variable will A, B, and b which are adsorbate specific, and

Table 5. Relative Sensitivity Parameters of the Input Variables

Parameter	Interval	Relative Sensitivity (%)
C0	$0.3 \le C_0/C_0 \le 0.6$	–515
	$0.3 \le C_0/C_0 \le 0.6$	–163
	$0.3 \le C_0/C_0 \le 0.6$	–52
W	$0.3 \le W/\overline{W} \le 2.0$	+120
R_p	$0.3 \le R_p/R_p \le 2.0$	–58

(iii) a further modification to the neural network that makes it of wide applicability to various fixed-bed adsorption scenarios is the inclusion of the particle size distribution. Many adsorption columns are multilayered; i.e., constructed of several layers of GAC (arranged in order) each having a different particle size. The HSDM model used in this study is a modified form which can take account of the particle size distribution [27]. The new input parameters that have to be added to the input layer are the fractions, from the total adsorbent weight W, of each particle size.

The neural network developed in this study has some advantages over the conventional mathematical models. Firstly, a prerequisite of constructing a mathematical model is the full understanding of the physical nature of the phenomenon under study. This, in many cases such as adsorption, is not achievable due to complexity of the problem. Hence, experimental observation is the only practical source of information regarding the physical phenomenon. Neural networks, on the other hand, have the ability to recognize the pattern involved in a certain phenomenon if they are trained on these observations. The variables thought to influence the physical process, and the primary desired output, are all that is needed to develop the network. Secondly, many complex physical phenomena, such as adsorption and filtration, require considerable computational effort and computer time if they are to be tested or simulated by mathematical models. On the other hand, a neural net that contains all connection weights can be run on a small personal computer. Moreover, the net can be easily translated into a small computer code that could be utilized by other users with a minimum knowledge in neural networks. Neural networks need to be trained on a large domain which covers most of the possible features related to a phenomenon. Therefore, neural networks can best be employed as interpolation tools where the data fall within the boundaries of the training domain. This can be considered one of the deficiencies associated with neural network as opposed to the mathematical models.

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Direct reprint requests to:

Professor Y. Najjar
Department of Civil Engineering
Seaton Hall
Kansas State University
Manhattan, KS 66506-2905