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Performance of a Virtual Adsorber System for Removal of Lead

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ABSTRACT

A granular activated carbon (GAC) column is an effective treatment technology for the removal of lead. However, this technology requires time-consuming and expensive bench- and pilot-scale studies to design a full-scale system. A virtual adsorber system (VAS) based on artificial neural network technology was developed from 67 bench-scale experiments as a new tool to optimize the GAC process. In addition, VAS can be used to design a full-scale adsorber system by eliminating the need for further lengthy and costly experiments. Data obtained from the VAS indicated that decreasing the influent lead concentration from 50 to 1 ppm increased the number of bed volumes (BVs) of wastewater treated at breakthrough from 30 to 950 BVs and exhaustion from 200 to 1650 BVs, while the surface loading decreased from 17 to 1.8 g Pb/g carbon. In addition, increasing the empty bed contact time from 1.85 to 12.75 minutes for each influent lead concentration increased the bed volumes of wastewater treated at breakthrough, while the bed volumes at exhaustion decreased and the surface loading slightly changed for the lower Pb concentration (1 and 10 ppm of Pb). Five sets of training data were selected to test the VAS. It was found that the VAS could predict the bed volumes at breakthrough and exhaustion, and surface loading with an accuracy of 97%. The average coefficients of correlation, R, between actual and virtual bed volume measurements at breakthrough and exhaustion and for surface loading were 0.988, 0.980, and 0.988, respectively, for the verification data, while they were 0.996, 0.994, and 0.996 for the training data. The high values of the correlation coefficients demonstrated the high performance of the VAS for the removal of lead.

INTRODUCTION

The presence of heavy metals in the environment is of concern because of their toxicity and threat to human life. In 1983 an estimated 7.9 billion gallons of heavy metals bearing wastewaters were generated in the United States (1). Recent attention to the impact of low-level lead on public health has encouraged a major research effort to develop effective means to identify, monitor, and remove lead from drinking water, wastewater, and groundwater. New regulations for lead in source and treated waters of public water systems, promulgated under the Safe Drinking Water Act amendments of 1986, require a source maximum contaminant level (MCL) of 0.005 mg/L.

Recently, activated carbon has been shown to remove lead from aqueous waste streams (2). Based on these results, an adsorber system such as a granular activated carbon (GAC) column may be an effective treatment technique for removal of heavy metals. However, it can be a relatively expensive process, especially if designed improperly. The proper design of full-scale adsorbers typically includes time-consuming and expensive pilot-scale studies. When regulations stipulate the maximum level for the contaminants, the design of an adsorber system to achieve these objectives requires the ability to predict the performance of the adsorbers.

Several adsorption and mathematical models are developed to describe the mechanisms of adsorption of heavy metals or organics by hydrous solids and GAC. These models are used by several researchers in an attempt to understand the parameters that limit the contaminant concentration within the water distribution system. In addition, the models are used to predict contaminant sorption into a GAC and to evaluate the performance of the adsorber system at the pilot- and full-scale level. These models are based on many assumptions. However, few of these models are totally satisfactory because they do not include all of the mechanisms that account for chemical spreading in fixed-bed adsorber systems.

Unlike predictive adsorption and mathematical models that require precise knowledge of all the contributing variables, artificial neural networks (ANN) can be a better tool to provide an understanding of how the adsorber system will respond under the various conditions expected in actual installations. The main objective of this study is to evaluate the performance of a virtual adsorber system (VAS) developed using ANN for the removal of lead.

BACKGROUND

Adsorption Mechanisms

Adsorption of a compound from a solvent to and into an adsorbent is usually described by a two-step process: 1) Transport through the film to

the outer surface of the particle, and 2) diffusion into the porous particle. The latter transport may be diffusion in the pore liquid or diffusion in the adsorbed phase. The adsorbed phase is assumed to consist of a layer of adsorbed molecules on the inner surface of the particles, the pore walls. The former mechanism is called pore diffusion and the latter surface diffusion. The rate of transport may be governed by either pore or surface diffusion or a combination of them besides the rate of transfer to the outer surface. Furthermore, the particles have a polydisperse pore structure, and the transport rate in pores of different sizes may not be equal. In very small pores, transport will be very slow due to spatial hindrances.

Mathematical Models

Adsorber dynamics in fixed beds such as GAC have been modeled using equilibrium theory, pseudomass transfer resistance, and both fluid- and adsorbent-phase mass transfer resistance to describe the adsorption rate.

Equilibrium Theory

The simplest approach is equilibrium theory. Equilibrium theory assumes that the adsorption rate is infinitely fast and provides asymptotic solutions to multicomponent fixed-bed adsorption models in the limit of rapid mass transfer rate. Furthermore, it can be used to estimate the order in which individual components in a mixture appear in adsorber effluents. However, equilibrium theory has limited application in the design and operation of fixed-bed adsorbers because mass transfer resistances are very important.

Pseudomass Transfer Resistance Models

These models describe the diffusion process by using simplified expressions. They give better descriptions of column data than equilibrium theory. However, many parameters in these simplified approaches come from model–data comparisons, and they are not capable of describing column data collected under a variety of conditions.

Mass Transfer Resistance Models

These models use pore or surface diffusive flux equations (Fick's law) for the intraparticle-phase mass transfer rate and the linear driving force approximation, and they are known as film transfer for the liquid-phase mass transfer rate.

Factors Affecting Metal Removal

Adsorption of heavy metal by activated carbon is a complex subject because it depends on the chemistry of water, the heavy metal specifica-

tions, and the chemistry of the carbon surface. Heavy metal removal by activated carbon is affected by removal kinetics, solution pH, ionic strength, competitive adsorption, and the adsorbate/adsorbent ratio.

Removal Kinetics

The removal of contaminants by activated carbon is a four-step process: bulk solution transport, film diffusion transport, pore transport, and adsorption. In bulk solution transport, the adsorbate is transported by diffusion from the bulk solution to the boundary layer of water surrounding the adsorbent particle. Film diffusion transport occurs by molecular diffusion though the stationary layer of water (hydrodynamic boundary layer) that surround particles. The boundary layer thickness is dependent on the rate of flow past the particle. Thus, a higher flow rate results in a smaller boundary layer. In pore transport the adsorbate is transported into and around the adsorbent's pores to available adsorption sites. Once the adsorbate has entered the pores, intraparticle transport may occur by molecular diffusion through the solution in the pores (pore diffusion) or by diffusion along the adsorbent surface (surface diffusion) after adsorption takes place. Adsorption occurs after transport to an available site. Adamson (3) reported the adsorption step to be rapid for physical adsorption; thus, the preceding diffusion will control the rate at which molecules are removed from solution. However, if adsorption is followed by a chemical reaction that changes the nature of the molecule, the chemical reaction may be slower than the diffusion step, by that means controlling the rate of compound removal.

Solution pH

The pH of the solution affects contaminant removal by influencing the surface charge of the activated carbon by affecting the distribution of the metal ions in the solution. As the pH decreases, the solubility of the metal generally increases. Sigworth and Smith (4) were among the first to report that adsorption of an inorganic by activated carbon depended on solution pH. The researchers showed that lead showed little adsorption at pH 2 but fairly good removal at pH 5. The onset of adsorption occurs before hydrolysis and precipitation of metals, and generally coincides with the loss of outer hydration covering of metal ions. It has been show that the adsorption density (mass of metal removed per unit mass of carbon) of Calgon Filtrasorb 400 increased with increasing pH to a maximum value and then declined rather rapidly with any further increase in pH for removal of chromium (5). When the pH was greater than 10, no appreciable adsorption was observed. Adsorption of cadmium on Nuchar SN carbon

peaked at approximately pH 6.7, followed by a decrease (6). However, the amount removed began to increase again at pH > 8.0 due to the resulting precipitation of cadmium from solution. Netzer and Hughes (7) found that adsorption of lead, cobalt, and copper was insignificant at pH < 2, but adsorption dramatically increased in the pH range from 4 to 10. Tan and Teo (8) reported that adsorption of lead by activated carbon was negligible at pH 1, but adsorption increased with increasing pH of the solution. The researchers also reported that lead removal was steadily increased between pH 5.5 and 11.5, but precipitation of white lead hydroxide was found to occur at higher pH values. At pH > 12, there was a reduction in lead removal due to the presence of PbO_2^- and $Pb(OH)_2^-$. Cadmium removal using two powered activated carbons (Nuchar SN and Darco HDB) was reported to be a strong function of solution pH (9). It was reported by Reed and Nonavinakere (10) that the extent of cadmium/nickel adsorption by three activated carbons (Darco KB, HD400, and Calgon F400) increased with increasing pH until a maximum was reached.

The fraction of metal removed from solution increases from a low value to nearly 100% in a narrow pH. This pH range is called the "pH-adsorption edge" and is specific to the heavy metal and carbon type. The adsorption-edge was from pH 3 to 7 for a majority of activated carbons. In general, adsorption gradually increases with increasing pH value until the onset of the adsorption edge is reached, after which adsorption increases significantly. Corapcioglu and Huang (11) reported that the adsorption edge of the lead species Pb(II) was between pH 3 and 6, and that pH was a dominant parameter because it affected the charge distribution of various species and the hydroxyl group distribution at the carbon surface.

Ionic Strength

Ionic strength and background electrolyte composition has been reported to affect metal removal by activated carbon. Huang and Smith (6) reported that cadmium removal decreased as ionic strength was increased from 0.01 to 0.1 M. Reed and Nonavinakere (10) studied the effect of ionic strength on metal adsorption by activated carbon. The researchers reported that metal removal decreased with an increase in ionic strength.

Competing Adsorbates

Generally, the adsorption capacity for heavy metals by activated carbon is reduced when more than one metal is present. Netzer and Hughes (7) reported that copper greatly affected the adsorption of cobalt. The adsorption capacity for lead was twice as much as that of copper and 10 times more than that of cobalt.

A competitive interaction has also been observed in the presence of organic compounds. Dolan (12) reported on the removal of a phenol and lead system by MWV-B activated carbon. An EBCT of 1.09 minutes was used. The feed solution contained either Pb(II) and phenol ($1.0 \times 10^{**}$ M) at a metal:ligand ratio of 1:1 or Pb(II) alone (1:0). Another reported that phenol removal was adversely affected by the presence of lead, but lead removal was unaffected by the presence of phenol.

Adsorbate/Adsorbent Ratio and Adsorbate Concentration

Metal removal by activated carbon in the batch mode depends on the concentration of solution per gram of carbon (adsorbate/adsorbent ratio). For the column mode the initial adsorbate concentration is important because the mass of carbon is constant. Tan and Teo (8) reported that the initial lead concentration greatly affects lead removal. The authors concluded that lead and chromium loading per gram of carbon (mg metal/g carbon) decreased with a decrease in adsorbate concentration.

Factors Affecting GAC Column Performance

Factors affecting GAC column performance include: empty bed contact time (EBCT), hydraulic loading rate (HLR), length of mass transfer zone (MTZ), and surface loading (X/M).

Empty Bed Contact Time (EBCT)

Netzer and Hughes (7) showed in batch studies that longer contact times were necessary for completed adsorption equilibrium when more than one metal was in solution with the carbon. The researchers concluded that this was related to the number of adsorption sites to the number of metal species in the solution.

The most important adsorber design parameter is the contact time or the EBCT. EBCT can be described by the following equation:

$$\text{EBCT} = V/Q = L_{\text{Bed}}/(Q/A)L_{\text{Bed}}/\text{approach velocity}$$

where V is the bulk volume of carbon in the adsorber, Q is the volumetric flow rate to the adsorber, L_{Bed} is the bed depth of carbon in the adsorber, and A is the cross-sectional area of the bed. The actual contact time is the product of the EBCT and intraparticle porosity, and this porosity usually ranges between 0.4 and 0.5 (13). EBCTs for GAC adsorbers range from a few minutes to more than 4 hours, depending on the contaminant types and concentrations.

EBCT has a significant impact on adsorber performance. For GAC column to yield any effluent of acceptable quality, the critical bed depth and the corresponding minimum EBCT must be exceeded. As the EBCT increases, the bed life (expressed in bed volumes of effluent to breakthrough point) of the adsorber increases until a maximum value is reached. Correspondingly, the carbon usage rate decreases to a minimum value. For a single adsorber, an optimum EBCT exists at which both the carbon usage rate and the efficiency are maximum. Increasing EBCT, or bed depth at a constant HLR, impacts the total treatment cost. As adsorber size increases, capital costs increase because of the increased costs of the larger systems. Operating and maintenance costs decrease because of decreasing carbon usage rate and replacement frequency.

Hydraulic Loading Rate (HLR)

The hydraulic loading rate can be defined as flow rate divided by the cross-sectional area of the column. Hydraulic loading rates vary from 0.4 to 12 gpm/ft^2, with a typical value being 2 to 4 gpm/ft^2. In column performance, the HLR can affect removal by varying the EBCT. Love and Eilers (14) performed several pilot-scale experiments to study the effect of increasing EBCT on bed life. A constant hydraulic loading rate of 3 gpm/ft^2 was for an influent of 18 ppb *cis*-1,2-dichloroethylene. As the EBCT was increased from 6 to 12 minutes, and then to 18 minutes, the number of bed volumes treated to a breakthrough concentration of 0.1 ppb was 4100, 7100, and 8100, respectively. The carbon usage rate for the 18-minute contact time is approximately one-half the value for the 6-minute contact time. Several authors have reported that increasing the L_{bed} at a constant HLR will affect annual treatment (15–17).

Mass Transfer Zone (MTZ)

The mass transfer zone (MTZ) is defined as the region of the activated carbon column in which adsorption is taking place. The activated carbon behind the MTZ is in equilibrium with the influent concentration ($C_e = C_0$). The region within the MTZ is where the adsorbent and adsorbate interact, and the degree of removal varies from 0 to 100%. This interaction is called "exhaustion," and the resulting surface loading as X/M (mg/g). The length of MTZ can be fixed for a given set of conduction, but $L_{critical}$ varies with the breakthrough concentration.

Surface Loading (X/M)

The surface loading (X/M) is related to column performance and can be defined as mass of adsorbate per mass of adsorbent. Unlike batch studies, the surface loading for columns is dependent on the initial adsorbate concentration (the mass of carbon is constant). The surface loading increased with increasing initial adsorbate concentration, resulting in a higher metal loading per gram of carbon.

Mechanics of a Neural System

In a typical neural data processing procedure, the data base is divided into two separate portions called training and test sets. Training set is used to develop the desired network. In this process (depending on the paradigm that is being used), the desired output in the training set is used to help the network adjust the weights between its neurons and processing elements (supervised training.) Once the network has learned the information in the training set and has "converged," the test set is applied to the network for verification. It is important to note that, although the user has the desired output of the test set, it has not been seen by the network. This is to ensure the integrity and robustness of the trained network. To clarify the actual functionality of a neural system, a short discussion on the mechanics and components of artificial neural network seems necessary. A fundamental understanding of theory and application of computational intelligence and neural networks specifically is essential in achieving meaningful results and repeatable outcomes.

In neural computing the artificial neuron is called a *processing element* or PE for short. The word *node* is also used for this simple building block. These artificial neurons bear only a modest resemblance to the real thing. They are barely a first-order approximations of biological neurons. Neurons in the human brain perform at least 150 different processes, whereas processing elements model approximately three of those processes. The PE handles several basic functions. It must evaluate input signals and determine the strength of each one. Next, it must calculate a total for the combined input signals and compare that total to some threshold level. Finally, it must determine what the output should be. Just as there are many inputs (stimulation levels) to a neuron, there should be many input signals to a PE. All of them should come into PE simultaneously. In response, a neuron either "fires" or "doesn't fire," depending on some *threshold* level. The PE will be allowed a single output signal; just as in a biological neuron—many inputs, one output.

In addition, just as real neurons are affected by things other than inputs, some networks provide a mechanism for other influences. Sometimes this

extra input is called a *bias term*, or a *forcing term*. It could also be a forgetting term, when a system needs to unlearn something. Each input will be given a relative *weighing* which will affect the impact of that input. This is similar to the varying synaptic strengths of biological neurons. Some inputs are more important than others in the way they combine to produce an impulse. Weights are adaptive coefficients within the network that determine the intensity of the input signal. One might think of them as a measure of the connection strength. The initial weight for a PE could be modified in response to various inputs and according to the network's own rules for modification.

Mathematically, the inputs and the weights on the inputs as vectors, such as $(I_1, I_2, \ldots, I_n)$ and $(W_1, W_2, \ldots, W_n)$ must be considered. The total input signal is the dot, or inner, product of the two vectors. The result is a scalar, not a vector. Geometrically, the inner product of two vectors can be considered a measure of their similarity. If the vectors point in the same direction, the inner product is maximum; if the vectors point in opposite directions (180°), their inner product is minimum. What was discussed before about signals coming into biological neuronal synapses applies here as well: signals can be positive (excitatory) or negative (inhibitory). A positive input promotes the firing of the PE, whereas a negative input tends to keep the PE from firing. If some local memory is attached to the PE, one can store results of previous computations and modify the weights used as the process continues. This ability to change the weights allows the PE to modify its behavior in response to its inputs, or *learn*. When weight adjustments are made in preceding layers of feed-forward networks by "backing up" from outputs, the term *backpropagation* is used. This is an important concept, because most networks today employ backpropagation algorithms.

Now, suppose that this processing element is combined with other PEs to make a layer of these nodes. Inputs could be connected to many nodes with various weights, resulting in a series of outputs, one per node. The connections correspond roughly to the axons and synapses in a biological system, and they provide a signal transmission pathway between the nodes. Several layers can be interconnected. The layer that receives the inputs is called the *input layer*. It typically performs no function other than the buffering of the input signal. The network outputs are generated from the *output layer*. Any other *layers* are called *hidden layers* because they are internal to the network and have no direct contact with the external environment. Sometimes they are likened to a "black box" within the network system. Although they are not immediately visible, one can examine what goes on in those layers. There may be zero to several hidden layers. The connections are multiplied by the weights associated with that

particular connection. They convey analog values. Note that there are many more connections than nodes. The network is said to be *fully connected* if every output from one layer is passed along to every node in the next layer.

Virtual adsorber system (VAS) presents a new and fresh approach toward soft experimentation with adsorber reactor systems such as granular activated carbon columns. The term soft experimentation is used to emphasize two points. First, word "soft" implies that instead of experimental laboratories, the process is carried out using a recently developed software (VAS). Second, the word "experimentation" is used to accentuate the high degree of accuracy (comparable to actual laboratory experiments) achievable using this software. It should also be noted that authors are not using the word "modeling" for their approach. This is due to the nature of the main tool used for VAS development, namely artificial neural networks. In using neural nets to mimic a process, no mathematical modeling takes place. Neural nets by definitions are model-free function estimators (18). They learn the process by observing its behavior, and estimate its functionality by adjusting the strength of network interconnections. Another factor that distinguishes the approach used in this study with mathematical modeling is the fact that during a mathematical modeling process two sets of information are essential for correct and accurate results. First is the number of parameters (variables) involved in the process and second is an accurate knowledge of the interrelationships (no matter how complex and nonlinear) between different parameters. When neural networks are used to build a function that estimates the process behavior, a complete knowledge of the above factors (all the parameters involved and their interrelationships) is not an absolute necessity. Using its massive connectivity, the neural networks can construct a high dimensional space through which accurate pattern recognition becomes possible. Another important point that recognizes neurocomputing from conventional mathematical modeling is its overall behavior. Even if a mathematical model of a certain process is available, its use is dependent on the accessibility of data and information on all involved variables in the model. A missing piece of information can cause the model to come to a halt. On the other hand, once a neural network is built to mimic a certain process, missing pieces of information will not cause an abrupt and total breakdown of the system. Because knowledge is distributed throughout the network, as opposed to a particular location, incomplete information, although it may jeopardize an accurate result, will not stop the whole process. As is known in neurocomputing circles, neural networks will "degrade gracefully."

MATERIALS AND METHODOLOGY

Experimental Procedures

The experimental work was conducted at the Environmental Engineering Laboratories of West Virginia University. GAC columns were operated in the upflow mode. The column setup schematic is presented in Fig. 1. Sixty-seven bench-scale experiments were carried out for the removal of lead from a synthetic wastewater using a GAC column. Lead nitrate was used as the source of lead for each experiment. The background electrolyte was sodium nitrate because it does not form complexes with lead. Wastewater pH was maintained at 5.4 to make sure the lead remained soluble. The pH was adjusted using nitric acid and/or sodium hydroxide. Parameters monitored during the experiment are presented in Table 1. Several different types of columns were used to achieve the specified empty bed contact times (EBCTs). The carbon was washed and sieved through a US No. 50 mesh sieve and added to the column by a slurry

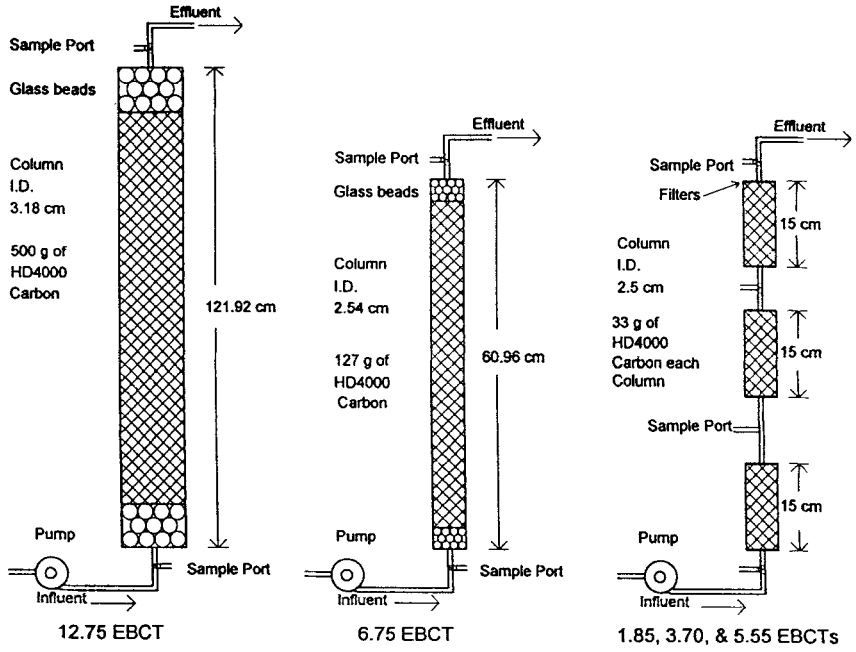

FIG. 1 Schematic of GAC column setup.

TABLE 1
Parameters Monitored for the VAS Development

Number	Parameter	Range
1	Mass of activated carbon	33–500 g
2	Length of column (cm)	15–122 cm
3	Diameter of the column (cm)	2.5–3.18 cm
4	Number of bed volumes treated per day	117–1556 BV/day
5	Number of regeneration	0–4 times
6	Concentration of lead (mg/L)	1–50 mg/L
7	Empty bed contact time (EBCT)	1.85–12.75 minutes
8	Hydraulic loading ratio (gpm/ft^2)	2–4 gpm/ft^2

method to avoid the presence of air bubbles. A variable speed Cole-Palmer pump was used to maintain the influent hydraulic loading rate. A carbon treatment step consisting of contacting the carbon columns with 10 bed volumes of 0.1 N HCl followed by 10 bed volumes of 0.1 N NaOH was employed for all the experiments. Several different influent concentrations of lead were investigated. The influent pH was maintained at 5.4, and sodium nitrate at an ionic strength of 0.01 N was used as a swamping electrolyte. Following each column run the carbon was regenerated using the same procedure as the pretreatment step. The acid rinse desorbed the lead and the base rinse reconditioned the carbon for the next run. For reproducibility, the experiments were repeated at least three times.

Lead samples were preserved by acidifying with concentrated nitric acid. The higher concentrations of lead were analyzed using a Perkin-Elmer Model 3100 ZL Atomic Adsorption (AA) spectrophotometer. The lower concentration (1 ppm) was measured with a Zeeman Atomic Adsorption Spectrometer. Criteria used to study the column performance include breakthrough bed volume, exhaustion bed volume, and surface loading. A schematic of the output data is presented in Fig. 2. A bed volume is the volume occupied by the carbon bed, including carbon volume and void volume. Breakthrough is the number of bed volumes treated when effluent concentration is 3% of influent concentration. Exhaustion bed volumes are the number volumes treated when effluent concentration is 95% of the influent concentration. Surface loading is the ratio of the mass (mg) of lead adsorbed on the carbon bed to the mass (g) of carbon in the column.

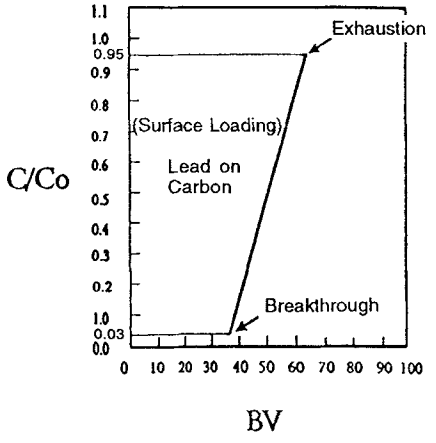

FIG. 2 Schematic of GAC column output data.

Neurocomputing Procedures

The bench-scale GAC column data was used to design and develop the virtual adsorber system (VAS). An ensemble of several neural networks was designed to mimic the experimental study. The compiled data were applied to the network, and the network parameters were tuned for optimum results. In Fig. 3 the architecture of the neural network designed for VAS is presented. The architecture, a fully connected network, included 240 synaptic connections (pertaining to a 240 dimensional hyperspace) between 13 input neurons, 15 hidden neurons, structured in a single layer and an output layer containing 3 neurons. Bipolar linear normalization was used in the input layer, and logistic function was used as the main activation function in the hidden and output layer neurons. Backpropagation of error was used as the training paradigm. The VAS was designed to predict bed volume at breakthrough, bed volume at exhaustion, and surface loading (ratio of the mass of contaminant to the mass of activated carbon) in a GAC column that removes lead from water. Eleven experiments called the verification samples were selected from the 67 bench-scale experiments. The remaining 56 laboratory experiments were chosen as the training data to train the neural network. Five sets of training data were selected to test the VAS. The organization of data samples for training and testing is presented in Table 2. The purpose of separating the verification samples was to test VAS's predictive capabili-

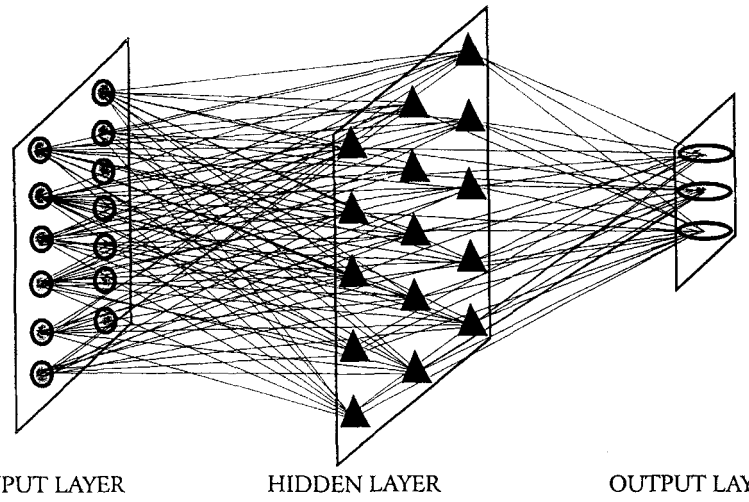

FIG. 3 Architecture of the neural network for the virtual adsorber system (VAS).

ties using an independent set of data. The performance of the final product (VAS) was based on how well the network could generalize what it had learned and how well it could predict the outcome of the contaminant removal process on a set of data it had never seen before.

RESULTS AND DISCUSSIONS

The results of the 67 bench-scale experiments were presented in previous papers (9, 10, 19, 20). In this paper the data were used to develop

TABLE 2
Organization of Data Samples for Training and Testing

Set	Testing set runs	Training set runs
1	R2, R14, R16, R18, R21, R27, R29, R32, R52, R62, R66	56 Runs selected from a total of 67
2	R1, R7, R11, R15, R22, R27, R32, R3246, R57, R59, R60	56 Runs selected from a total of 67
3	R20, R21, R25, R29, R31, R43, R51, R62, R64, R65, R66	56 Runs selected from a total of 67
4	R2, R8, R20, R22, R30, R32, R48, R49, R60, R63, R66	56 Runs selected from a total of 67
5	R1, R5, R21, R41, R43, R48, R51, R52, R53, R66, R68	56 Runs selected from a total of 67

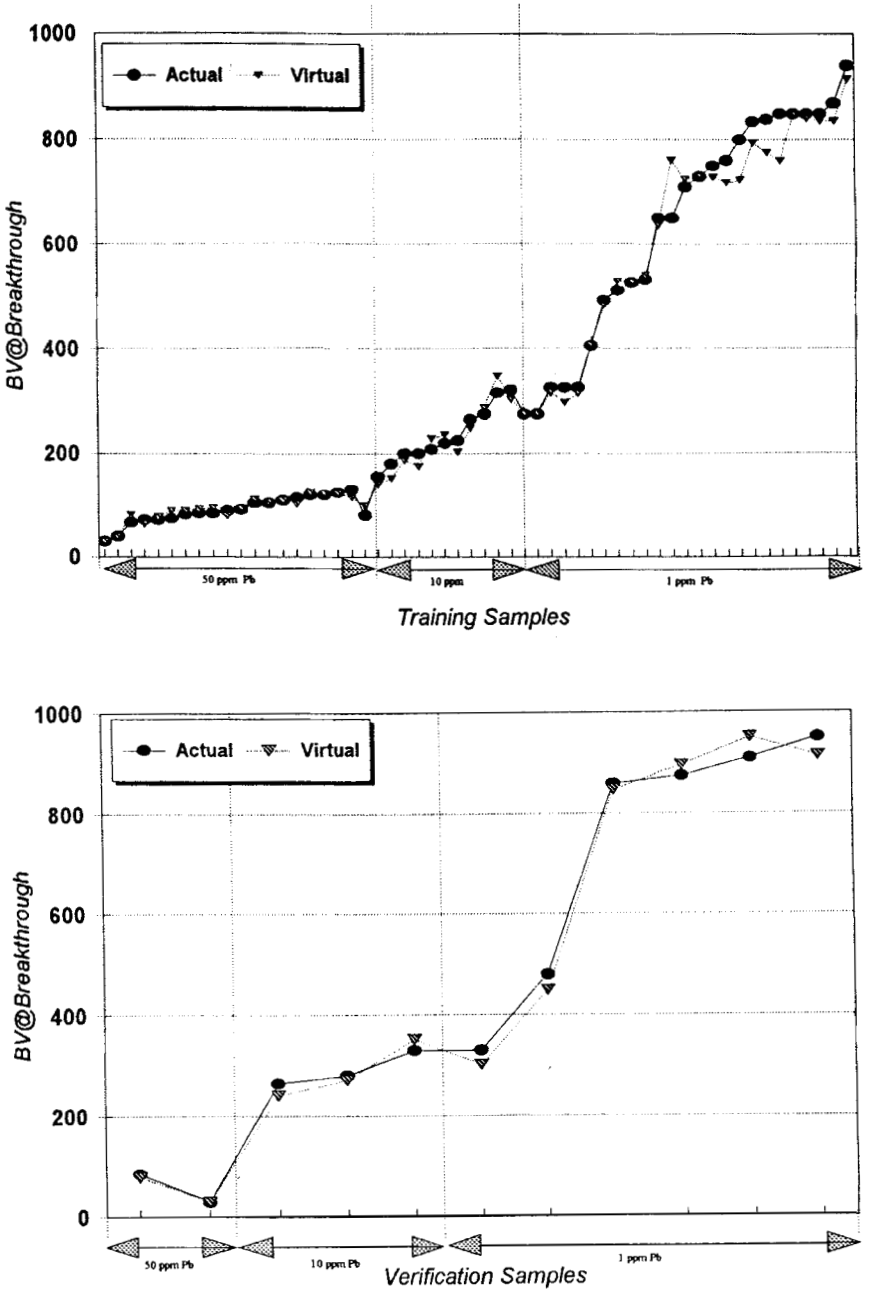

FIG. 4 Actual and virtual measurement of breakthrough.

and evaluate the performance of the VAS for removal of lead. The artificial neural network (using a supervised training paradigm) was trained with a set of data (training data) that included the pair of input and the corresponding output values. The weight (strength) of the connections between neurons were initialized and the training started by exposing the network to one set of the input data (input–output pair) at a time. As the network observed the input–output pair, it adjusted the weights of its connections to capture different features presented in the training data. Some convergence criteria were set for reaching acceptable results. Once the convergence was achieved, the network had reached a stable state. At this point the network had extracted all the necessary information from the training data and had established a complex pattern between input and output variables. Information and knowledge were encoded in the form of stable states or mapping embedded in the network. Once this step was completed, the network was ready to recognize any pattern related to the problem. Five sets of training data were used to test the VAS. Actual and virtual measurement of bed volume (BV) at breakthrough, exhaustion, and the surface loading data for both the training data and verification samples are presented in Figs. 4, 5, and 6, respectively. Please note that these figures represent only the data set 2. As observed, the VAS results indicated that decreasing the influent lead concentration from 50 to 1 mg/L (ppm) increased the number of bed volumes (BVs) of wastewater treated at breakthrough from 30 to 950 BVs and at exhaustion from 200 to 1650 BVs. The surface loading was noticed to decrease from 17 to 1.8 g Pb/g carbon. In addition, increasing the empty bed contact time (EBCT) from 1.85 to 12.75 minutes for each influent lead concentration increased the bed volumes of wastewater treated at breakthrough but decreased the bed volumes at exhaustion, while the surface loading slightly changed for the

TABLE 3
Coefficients of Correlation for Test and Training

	Coefficients of correlation, R					
	BV at breakthrough		BV at exhaustion		Surface loading	
Set	Test	Training	Test	Training	Test	Training
1	0.998	0.996	0.990	0.995	0.990	0.994
2	0.991	0.999	0.960	0.999	0.998	0.999
3	0.967	0.996	0.996	0.995	0.979	0.998
4	0.991	0.995	0.966	0.994	0.990	0.997
5	0.994	0.993	0.988	0.988	0.984	0.994

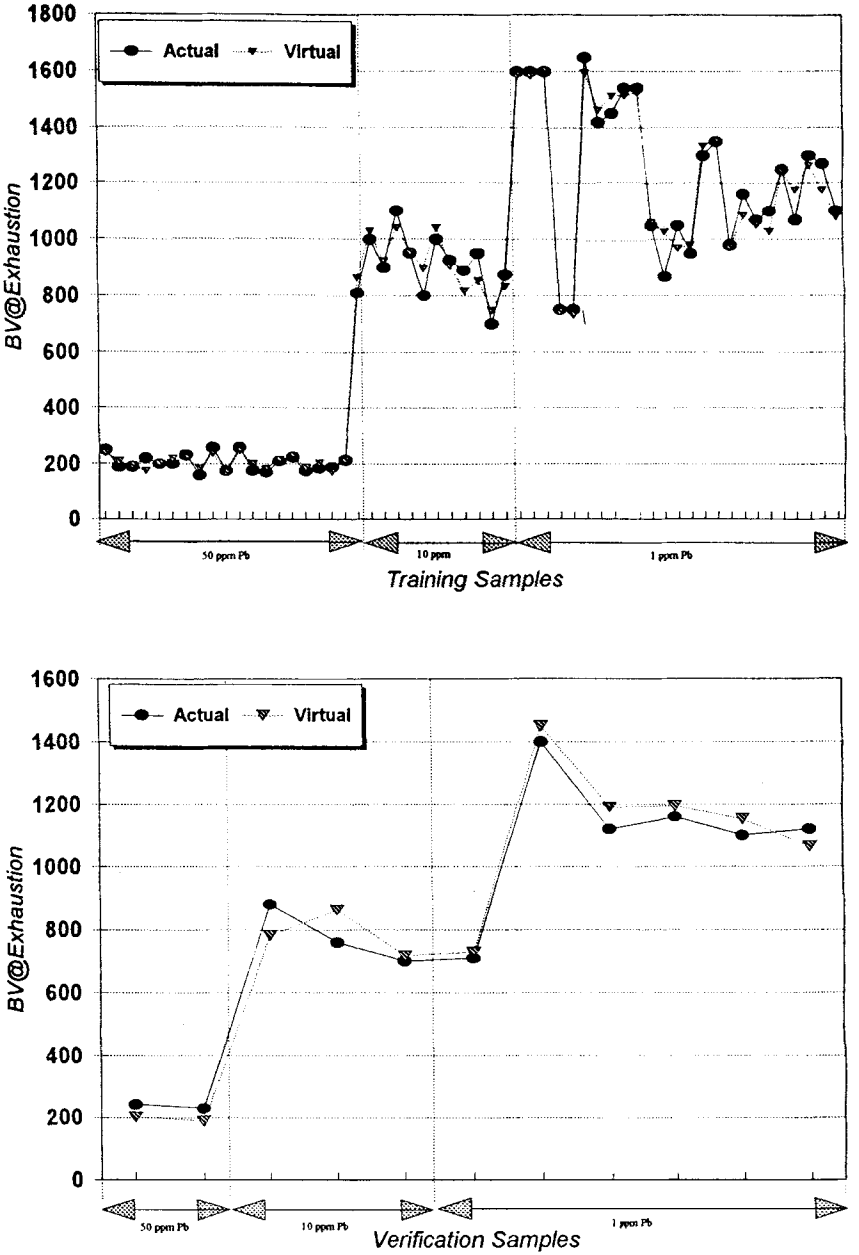

FIG. 5 Actual and virtual measurement of exhaustion.

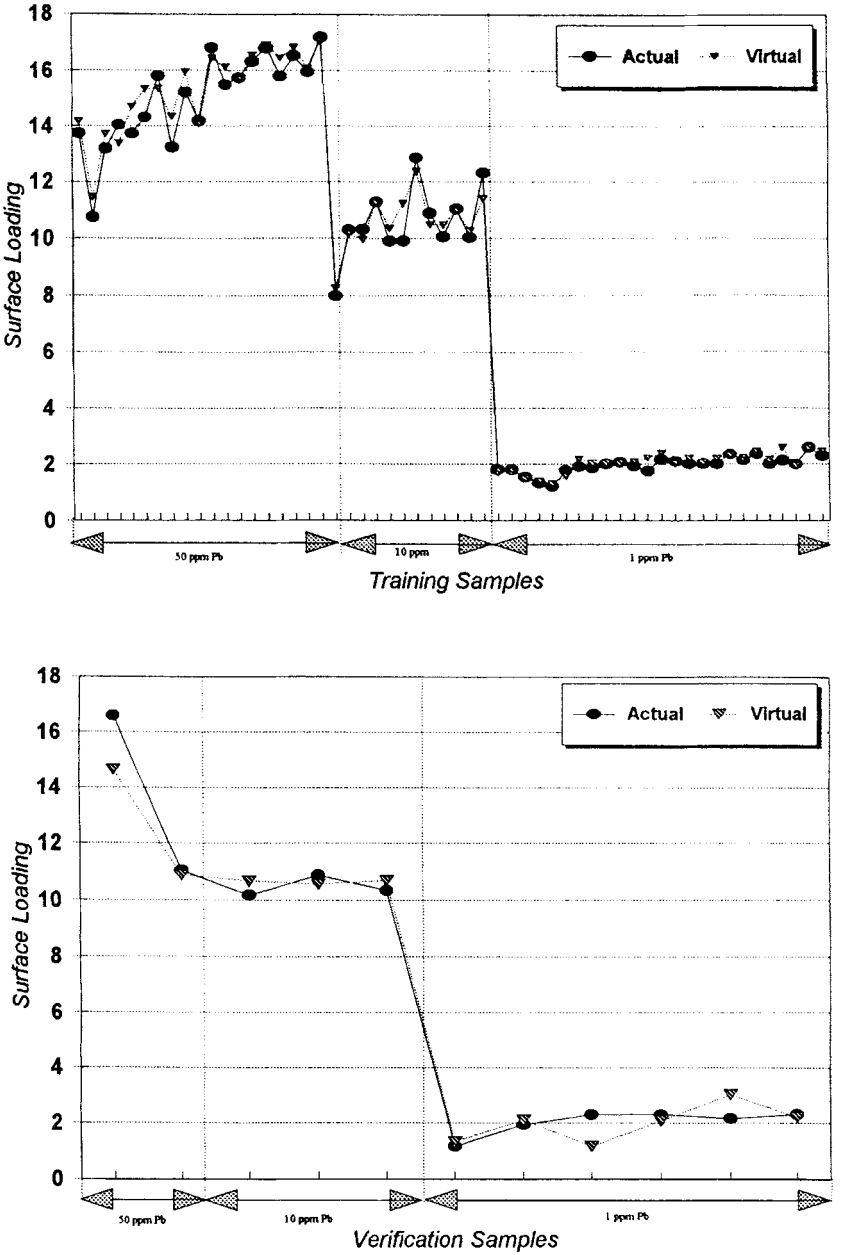

FIG. 6 Actual and virtual measurement of surface loading.

lower Pb concentration (1 and 10 mg/L of Pb). Clearly the network had learned the training data well and could reproduce the experimental results that it had been trained on with accuracies of about 97%. The correlation coefficients, R, for the five training sets of data obtained from the VAS software are presented in Table 3. The average coefficients of correlation for bed volumes at breakthrough and exhaustion and for surface loading are 0.996, 0.994, and 0.996, respectively.

The bottom graphs in the aforementioned figures (verification samples) test the generalization power of the developed VAS. A degree of accuracy of 96% could be achieved for the five test sets. The correlation coefficients, R, for the five verification samples data obtained from the VAS software are presented in Table 3.

The VAS software provided very accurate values for bed volumes at breakthrough, bed volumes at exhaustion, and surface loading for sets of input data (experimental conditions) that it had never seen before. The average coefficients of correlation for bed volumes at breakthrough and exhaustion and for surface loading are 0.988, 0.980, and 0.988, respectively.

CONCLUSIONS

Granular activated carbon (GAC) column data on lead removal in aqueous system were collected from 67 bench-scale experiments to develop the virtual adsorber system (VAS) based on artificial neural network (ANN) technology. The data obtained from the VAS indicated that decreasing the influent lead concentration from 50 to 1 ppm increased the number of bed volumes (BVs) of wastewater treated at breakthrough from 30 to 950 BVs and exhaustion from 200 to 1650 BVs, but decreased the surface loading from 17 to 1.8 g Pb/g carbon. In addition, increasing the empty bed contact time (EBCT) from 1.85 to 12.75 minutes for each influent lead concentration increased the bed volumes of wastewater treated at breakthrough but decreased the bed volumes at exhaustion, while the surface loading slightly changed for the lower Pb concentration (1 and 10 ppm of Pb). Five sets of training data were used to test the VAS. It was found that the VAS could predict the bed volumes at breakthrough and exhaustion and for surface loading with an accuracy of 97%. The average coefficients of correlation, R, between actual and virtual measurements of bed volumes at breakthrough and exhaustion and for surface loading were 0.988, 0.980, and 0.988, respectively, for the verification data, while they were 0.996, 0.994, and 0.996 for the training data. The high values

of the correlation coefficients demonstrated the high performance of the VAS for removal of lead.

The outcome of this study can be used to help engineers in selecting the best combination of parameters for heavy metal treatment and help them in designing the process by eliminating the need for further lengthy and costly experimentations. The main characteristics of VAS are that unlike conventional approaches based on rigorous mathematical models, there is no attempt in VAS to mathematically model the decontamination process. This is an advantage of the process being introduced in this study.

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