Desalination and Water Treatment
www.deswater.com

doi: 10.1080/19443994.2014.987172

57 (2016) 3632–3641
February

Taylor & Francis
Taylor & Francis Group

Artificial neural network modelling for removal of chromium (VI) from wastewater using physisorption onto powdered activated carbon

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Received 3 March 2014; Accepted 7 November 2014

ABSTRACT

A three-layered feed-forward artificial neural network (ANN) model has been designed to predict the adsorption efficiency and adsorption capacity for the adsorptive removal of chromium (VI) from synthetic wastewater. The adsorbent dose, wastewater pH, initial pollutant concentration and contact time were used to develop the network. The data used to train and test the model were obtained from several batch experiments. Various algorithms and transfer functions for hidden layer were tested to find the most reliable network. Broyden–Fletcher–Goldfarb–Shanno (BFGS) quasi-Newton backpropagation algorithm gave the most satisfactory results for adsorption efficiency. Resilient and BFGS quasi-Newton backpropagation were the most suitable algorithm for adsorption capacity. The best combination of training algorithm and transfer function for adsorption efficiency was found to be trainrp and poslin, while poslin produced simulated results within 10% deviation for adsorption capacity. Eight to eleven neurons were found to be optimum using trial-and-error method. The ANN predicted and experimentally measured values were compared to test the accuracy of the model.

Keywords: Wastewater treatment; Adsorbent; Adsorption; Artificial intelligence; Automation

1. Introduction

Great efforts have been made in recent years to develop suitable technologies for efficient removal of chromium (VI) from wastewater which is reported to be one of the top 16 toxic pollutants to date [1]. Adsorption, due to its operational easiness, design simplicity, cost-effectiveness and robustness [2], has been studied extensively over other contemporary techniques such as precipitation, coagulation, flocculation, ion exchange, photocatalytic degradation, solvent extraction, membrane separation, biological processes, sonochemical degradation and integrated treatment for the removal of chromium (VI) from wastewater. Nevertheless, adsorptive removal of chromium (VI) from wastewater can further be upgraded through automation, since automation of wastewater treatment processes is essential to make their operation easier, saving manpower and energy [3]. However, the development of an

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automated wastewater treatment plant is very difficult as the parameters of industrial effluents change severely thus leading to drastic change in output of treatment plant. Particularly, talking about adsorption, its dynamic characteristics are very complicated [4].

This complication leads to poor interpretation and quantification of interactions between process inputs and outputs and thus it becomes arduous to describe non-linear behaviours of a wastewater treatment plant through linear mathematical models [5,6]. Therefore, a computer-simulated model is required for interrelating the input and output parameters. The conventional analysis using regression technique is not suitable for adsorption experimental data since the technique fails to understand the physics of the system [7]. Recently, response surface methodology has also been implemented to model numerous processes in chemical, environmental and bioresource engineering; however, artificial neural network (ANN) has proven to be a superior and more accurate modelling technique [8]. Neural network-based models provide a better alternative to statistical models because of their computational efficiency, generalization ability and capability to handle data having high dimensionality [9]. More specifically, the ANN model gives better results for predicting results from adsorption database [10], describe adsorption systems better than general rate models [11] and even represent the adsorption isotherms [12]. Thus, ANN can be used efficiently to develop the model which can be coupled with model predictive control system for automotive or online monitoring of effluent treatment plant containing toxic pollutants.

ANNs have been implemented for modelling water treatment processes such as ultrafiltration, anaerobic biological treatment, activated sludge process, chlorination, advanced oxidation process, coagulation, flocculation and sedimentation commonly used in effluent treatment industries. They are also used to predict optimal alum doses, water-quality index, biochemical oxygen demand, chemical oxygen demand, colour, biological oxygen demand, suspended solids, removal of phosphorus, phenolic compounds, etc. However, there is no model using ANNs aimed at predicting chromium (VI) removal from wastewater using adsorption onto powdered activated carbon. Hence, the aim of this manuscript is to present the design; execution and assessment of ANN approach towards the treatment of highly polluted effluents containing chromium (VI). The detailed objectives of this paper are: to develop ANN models that are capable of predicting adsorption capacity and adsorption efficiency for removal of chromium (VI) from aqueous solution; and to implement the ANN models so that they can be used efficiently for automation of chromium (VI)-containing effluent treatment plant and thus can be used easily by operators of such plants.

2. Experimental section

2.1. Materials

Resources mainly required to perform the experiments included powdered activated carbon as adsorbent and chemical reagents to prepare synthetic wastewater solution. The powdered activated carbon (CAS No. 1440-44-0) chosen as adsorbent in this study was procured from Merck, India. Various characteristics and properties of this activated carbon as provided by the manufacturer are: molar mass 12.01 g/mol; melting point 3,550°C; bulk density 150–440 kg/m^3; and methylene blue adsorption ≥80 mg/g. This adsorbent also contained chloride ≤0.2%; sulphate ≤0.2%; heavy metals ≤0.005%; iron ≤0.1%; substances soluble in water ≤1%; and substances soluble in hydrochloric acid (HCl) ≤3%. Chemicals required in preparing synthetic wastewater and related experimental works comprised of potassium dichromate ($K_2Cr_2O_7$), sulphuric acid (H_2SO_4), 1, 5-diphinylcarbazide (DPC), HCl, sodium hydroxide (NaOH) and acetone (C_3H_6O). All these chemicals purchased from Merck, India were of analytical reagent grade and used without further purification.

2.2. Simulated wastewater preparation

Chromium-containing wastewater for laboratory-scale experiments is prepared through mixing a chemical compound having the desired oxidation state of the metal under consideration in the distilled water. A reserve wastewater feed containing chromium (VI) 1,000 mg/L was prepared by dissolving the necessary amount of $K_2Cr_2O_7$ in distilled water. The stock solution was diluted as required to obtain solutions of concentrations ranging between 10 and 250 mg/L. The pH levels of wastewater were adjusted by adding necessary quantity of HCl and NaOH. The ultrapure deionized water (18.2 MΩ cm resistivity at 25°C and <4 ppb total organic carbon) used in this study was obtained from Arium 611DI ultrapure water system (Sartorius A.G., Gottingen, Germany). The feed to this Arium 611DI water purification system was taken from usual laboratory distillation unit.

2.3. Experimental procedure

The effects of process parameters such as pH, initial chromium (VI) concentration, contact time, activated

carbon dose and temperature on the adsorption efficiency and adsorption capacity were evaluated using the batch experiments carried out with six different concentrations of chromium (20, 50, 100, 150, 200 and 250 ppm), different adsorbent dosage (0.5–2.0 g/L), six different temperatures (5, 10, 25, 30, 40°C), pH levels (1.5–8) and contact time intervals (0–110 min). The solutions were stirred using laboratory-scale magnetic stirrer in covered beakers which worked as adsorbers. Samples during the adsorption experiment were collected with time and concentrations of chromium (VI) were measured. Significant pH drift was studied by measuring pH at initiation and termination level of each experimental run. This magnetic stirrer apparatus operates on 220/230 V AC. The temperature of the solution was maintained using a constant temperature water bath. The speed of the stirrer was maintained at 150 rpm. The slurries were filtered through Whatman filter papers and the equilibrium concentrations were determined by Hitachi dual beam a UV–visible spectrophotometer.

2.4. ANN modelling

ANN is a technique animated by the design of biological nervous systems whose ith neuron has input value x_i, output value $y_i = f(x_i)$ and connections with the other neurons are expressed by weights w_{ij} [9]. Advantages of ANN model over traditional mathematical models include: inessential complex mechanism of the process, lesser simulation time for model development and less-extensive experimentation [13,14]. The ANN network configuration consists of three layers, namely input layer, hidden layer and output layer. The input layer collects the input variables, processes it to the hidden layer and the output layer delivers the ANN-predicted response. Each layer has a number of nodes called neurons connected together by a communication line called connection. Each neuron takes many input signals and based on an assigned weight value, produces a single output signal, which is typically sent as input to another neuron [15]. The nodes of the hidden layer enhance the ability of ANN to model complex relationships [16]. The number of hidden nodes depends on the number of training patterns, the amount of data noise and the complexity of the function that ANN is approximating [17]. The three layers considered in this work are shown in Fig. 1. The input variables selected to develop the model are batch time, pH of the solution, initial solute concentration and adsorbent dose, whereas adsorption efficiency and adsorption capacity are the output variables.

The majority of the ANN applications involve the utilization of feed-forward (FF) and backpropagation (BP) method to train the neural networks [18,19]. The performance of the FF is considered to be superior to conventional statistical and stochastic methods [20,21] and BP is contemplated as the most effective algorithm for adjusting the weights of a multi-layered neural network [22]. In this study also, ANN model has been calibrated using FF-BP method. Six BP algorithms were compared to select the best-fitting BP algorithm for the gathered data. For all algorithms,

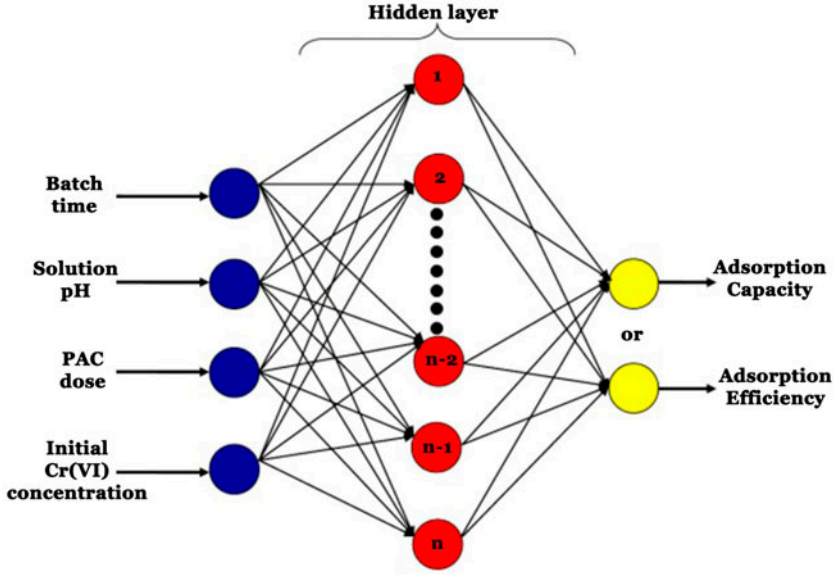

Fig. 1. Schematic diagram of ANN model with four inputs and one output layer.

different transfer functions, namely tansig, satlin and poslin at the hidden layer and purelin transfer function at the output layer, were used. The mathematical explanations of different transfer functions used are given in Table 1. The learning rate of the network was adjusted so that training time was minimized. MATLAB 7 (The MathWorks, Inc) was used to develop these ANN models.

3. Results and discussion

3.1. Selection of adsorbent

There are numerous activated carbons derived from agricultural, industrial and municipal wastes which have been utilized by researchers to study adsorptive removal of chromium (VI) from wastewater. Mohan and Pittman Jr. [23] presented a state of the art review on remediation of chromium (VI) from water using activated carbons prepared from precursors such as rice bran, saw dust, coir pith, soybean hulls, sugarcane bagasse, corn stover, saltbush, groundnut shell, walnut shell, almond shell, *Terminalia arjuna* nuts, natural organic wastes, sludge, industrial wastes, hazelnut shell, *T. indica* seed, *A. flavus*, etc. Though these activated carbons are of low cost and renewable, however, the greatest problem with these precursors is their unavailability in the global market and inability to meet the commercial demand due to huge consumption of activated carbons; hence, industries have to depend on the commercial activated carbons [24]. Since the aim of this paper is to construct ANN model for the development of automated chromium (VI)-containing wastewater treatment plant for which high-removal efficiency and adsorption capacity is sought, hence commercial activated carbon was chosen for the experimental runs. Various authors have reported efficient performance of commercial activated carbons for the removal of chromium (VI) from wastewater [25–27].

Table 1
Mathematical expressions of the transfer functions used for the hidden layer

Transfer functions	Mathematical expression
purelin	purelin (n) = n, for all n
tansig	tansig (n) = $2(1 + \exp(-2n)) - 1$
satlin	satlin (n) = 0, if $n \leq 0$ = n, if $0 \leq n \leq 1$ = 1, if $1 \leq n$
poslin	poslin (n) = n, if $n \geq 0$ = 0, if $n \leq 0$
logsig	logsig (n) = $1(1 + \exp(-n))$
n is any variable	

3.2. Selection of input parameters

Selection of input variables from a number of parameters that affect the process is a significant segment for configuration and performance of neural network though the selection method may be extremely protracted [28]. The inputs should be selected in such a careful manner that they reflect the fundamental of the process and the model developed from them should represent the whole ranges of operating conditions consistently [29]. Batch adsorption experiments were carried out to select various significant factors influencing the adsorptive removal of chromium (VI) from simulated wastewater. Effects of various parameters on the removal of chromium (VI) from wastewater over powdered activated carbon have been studied in our previous work [24]. It was observed that the adsorption was favourable at acidic condition and adsorption capacity decreased with increasing pH. The removal of chromium (VI) increased with increasing adsorbent concentration and the adsorption capacity increased with increasing initial chromium (VI) concentration and as the contact time increased, the rate of adsorption decreased. However, the effect of temperature was not prominent. Hence, the network has been modelled considering four input parameters viz. pH of wastewater, adsorbent dose, initial chromium (VI) concentration and contact time, whereas the adsorption capacity and adsorption efficiency is an output parameter of the ANN model. The use of simpler models with fewer numbers of parameters is usually preferable to those with more parameters whenever feasible [30]. Experimental data-set at different operating conditions were used to train and test the neural network model. The ranges of different operating parameters are given in Table 2. It is worth mentioning that the ranges

Table 2
Ranges of different operating parameters used for experimental run

Input parameters	Range of parameter value
pH	2–8
PAC dose (mg/L)	0.5–2
Initial Cr(VI) concentration (mg/L)	50–250
Time (min)	0–110

considered for the four variables under investigations were chosen based on the available literature as well as the experiments previously performed by the authors.

3.3. Optimization of neural networks

The optimum design of a neural network is central for its perfect and effective application. There are several parameters such as network type, network architecture, training algorithms, activation functions, input selection, neural network weight, momentum rate, number of iterations and data-set partitioning ratio which influence the ANN model [28]. However, all algorithms and transfer functions may not be applicable for all the processes. Selecting an appropriate training algorithm, transfer function and number of neuron in all layers are very sensitive parameters for network design as they have a significant impact in network training performance, training time and its generalization abilities. Training of the neural networks is sensitive to the number of neurons in the hidden layer. The more the number of neurons, the better is the performance of the neural network in

Table 3
Trial-and-error results for development of adsorption efficiency ANN model

Algorithm	Function	Hidden layer transfer function	Output layer transfer function	Correlation coefficient	Remark
Conjugate gradient backpropagation with Polak–Ribiere updates	traincgp	tansig	purelin	Too low	Arbitrary results
		satlin		Too low	Arbitrary results
		poslin		Too low	Arbitrary results
Levenberg Marquardt backpropagation	trainlm	tansig	purelin	Too low	Arbitrary results
		satlin		Too low	Arbitrary results
		poslin		Too low	Arbitrary results
Gradient descent with momentum and adaptive learning rate backpropagation	traingdx	tansig	purelin	Too low	Arbitrary results
		satlin		Too low	Arbitrary results
		poslin		Too low	Arbitrary results
Resilient backpropagation	trainrp	tansig	purelin	0.82	Unsatisfactory results
		satlin		Too low	Arbitrary results
		poslin		0.78	Unsatisfactory results
BFGS quasi-Newton backpropagation	trainbfg	tansig	purelin	Too low	Arbitrary results
		satlin		Too low	Arbitrary results
		poslin		0.96	Satisfactory results
Scaled conjugate gradient backpropagation	trainscg	tansig	purelin	0.79	Unsatisfactory results
		satlin		Too low	Arbitrary results
		poslin		Too low	Arbitrary results

fitting the data. However, it must be taken into account that presence of numerous neurons in the hidden layer may be the cause for over-fitting [31] which may lead to the loss of generalization capability of network, besides, small number of neurons in hidden layer may under fit the data, and subsequently the network may not be able to learn. Thus, if the model does not comply with the experimental results, then the output value from water treatment plant will be haphazard and it will be difficult to control the plant. Trial-and-error method was followed to find the most suitable network model, the optimum number of hidden layers and the optimum number of neurons in the hidden layer [32]. The maximum number of hidden layers considered was one. Inclusion of more hidden layer will increase the complexity of the system and consequently the time and cost of simulation. Researchers have proved that a network with one hidden layer can approximate any continuous function if degrees of freedom are sufficiently provided [33]. To reach the suitable network architecture, several trials for each group have been conducted until the suitable learning rate, number of hidden layers and number of neurons per each hidden layer was reached. The suitable architecture is the one which produced the minimal error term in both training and testing data. The performance of each network model is evaluated by computing the MSE for each trial conducted in search of the suitable architecture. It has been found that FF network and 8–11 neurons produce minimum value of MSE, so all models were designed and tested with 10 neurons. Simulated data was comparatively studied with one low, one medium and one in high-value range experimental points to test and validate the network model.

3.4. Adsorption efficiency model

Adsorption efficiency refers to the performance of adsorption process in removing the pollutant under consideration for a given set of operating parameters. It may also be termed as removal efficiency. Our previous experiments found that under optimum conditions of wastewater pH, adsorbent dose and contact time 100% removal of chromium (VI) was possible [24]. Mathematically, the adsorption efficiency is determined using the following relation: $R = [(C_o - C_f)/C_o] \times 100$; where R is the percentage removal of pollutant, C_o is the initial concentration of solute (mg/L) and C_f is the final concentration of solute (mg/L). This equation was used to develop the adsorption efficiency model. Various algorithms and transfer functions used to construct the adsorption efficiency neural network were repeated 10 times to train the network and the values of correlation coefficients were taken into account from the best of 10 repeated runs [34]. The outcomes of trial-and-error method adopted to formulate the adsorption capacity neural network as discussed earlier are shown in Table 3. Number of iteration varied in each run. The maximum termination criteria were fixed at iteration number 300; however, it reached the error criteria i.e. 10^{-2} within 180–250 iterations. Time taken for each run was 3–4 s.

It is apparent from the table that the correlation coefficient associated with "satlin" transfer function for hidden layer is too low and gives arbitrary results in each case. The "tansig" transfer function also exhibited too low correlation coefficients and gave arbitrary results in maximum cases. Though with "Resilient" and "Scaled conjugate gradient" BP algorithm showed correlation coefficients of 0.82 and 0.79, respectively, the results were non-satisfactory. The "poslin" transfer function too gave very low values of correlation coefficients and arbitrary results in many cases. It showed significant correlation coefficient with "Resilient" BP algorithm and "trainrp" function; however, results were not satisfactory. The best and most suitable combination of training algorithm and functions for adsorption efficiency computation was found to be "BFGS quasi-Newton" backpropagation algorithm, "trainbfg" and "poslin" with the corresponding correlation coefficient 0.96. Fig. 2 compares experimental adsorption efficiencies with the predicted values obtained from the adsorption efficiency neural network model using the most appropriate combination that is BFGS quasi-Newton backpropagation algorithm with poslin transfer function. The figure demonstrates good agreement between

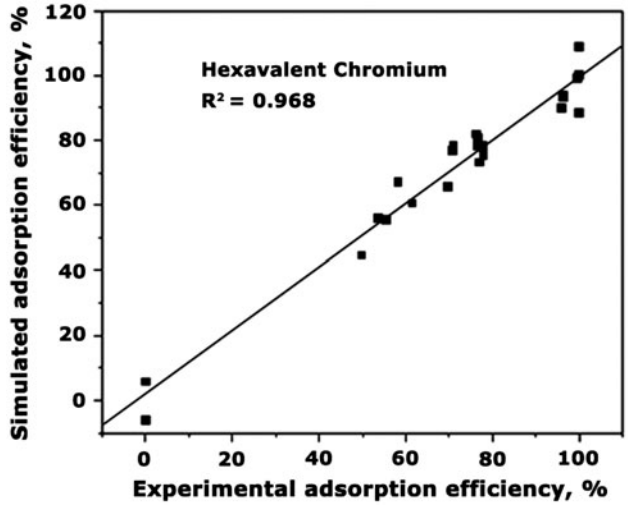

Fig. 2. Simulated result vs. experimental result for adsorption efficiency ANN model.

the experimental and predicted values as *R*-Squared value 0.968 for the line is very much close to the unity.

3.5. Adsorption capacity model

Adsorption capacity is a term associated with the adsorbent which denotes the competence of an adsorbent material towards adsorption of a solute at a given set of operating conditions. It is also an inherent characteristic of the adsorbent material which depends on the precursor and conditions used to prepare them. The capacity of an adsorbent for a given initial concentration of the adsorbate depends on the adsorbent dosage. Mathematically, adsorption capacity is determined using the relation: $Q = [(C_o - C_e)\ V]/W$; where Q is the adsorption capacity (mg/g), C_o is the initial concentration of solute (mg/L), C_e is the equilibrium concentration of solute (mg/L), W is the weight of adsorbent (g) and V is the volume of wastewater taken (L). This equation was used to develop the adsorption capacity model. The adsorption capacity model was simulated with different algorithms and transfer functions. The outcomes of trial-and-error method adopted to formulate the adsorption capacity neural network as discussed earlier are shown in Table 4.

Table 4
Trial-and-error results for development of adsorption capacity ANN model

Algorithm	Function	Hidden layer transfer function	Output layer transfer function	Correlation coefficient	Remark
Conjugate gradient backpropagation with Polak–Ribiere updates	traincgp	tansig	purelin	Too low	Arbitrary results
		satlin		Too low	Arbitrary results
		poslin		0.76	Unsatisfactory results
Levenberg Marquardt backpropagation	trainlm	tansig	purelin	Too low	Arbitrary results
		satlin		Too low	Arbitrary results
		poslin		0.81	Unsatisfactory results
Gradient descent with momentum and adaptive learning rate backpropagation	traingdx	tansig	purelin	Too low	Arbitrary results
		satlin		Too low	Arbitrary results
		poslin		0.78	Unsatisfactory results
Resilient backpropagation	trainrp	tansig	purelin	0.83	Unsatisfactory results
		satlin		Too low	Arbitrary results
		poslin		0.96	Satisfactory results
BFGS quasi-Newton backpropagation	trainbfg	tansig	purelin	Too low	Arbitrary results
		satlin		Too low	Arbitrary results
		poslin		0.97	Satisfactory results
Scaled conjugate gradient backpropagation	trainscg	tansig	purelin	0.83	Unsatisfactory results
		satlin		Too low	Arbitrary results
		poslin		0.79	Unsatisfactory results

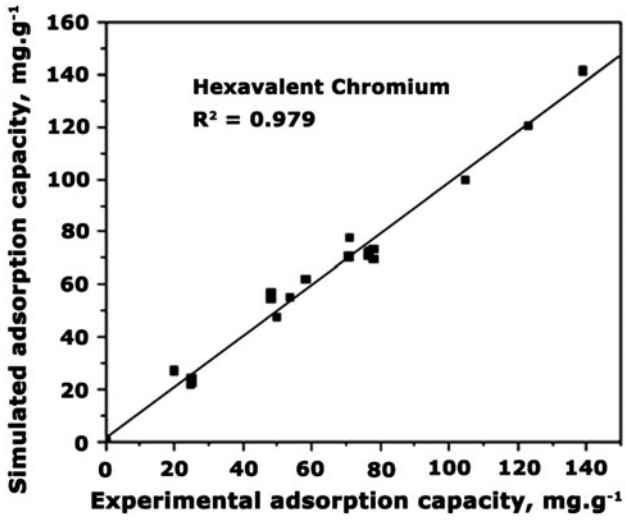

Fig. 3. Simulated result vs. experimental result for adsorption capacity ANN model.

It is evident from the table that the correlation coefficient associated with "satlin" transfer function for hidden layer is too low and gives arbitrary results in each case. The "tansig" transfer function also exhibited too low correlation coefficients and gave arbitrary results in maximum cases. Though with "Resilient" and "Scaled conjugate gradient" BP algorithm it showed 0.83 value of correlation coefficient, the results were non-satisfactory. It is the "poslin" transfer function that gave the most suitable and satisfactory results for adsorption capacity model in combination with Resilient BP and BFGS quasi-Newton BP algorithms with correlation coefficient values 0.96 and 0.97, respectively. Resilient backpropagation algorithm with transfer function poslin produced simulated results within 10% deviations during test and validation similar to that reported in the literature [34]. Fig. 3 compares experimental adsorption capacities with the predicted values obtained from the adsorption capacity neural network model using the most appropriate grouping viz. "Resilient" BP algorithm with "poslin" transfer function. The figure demonstrates good agreement between the experimental and predicted values as *R*-Squared value 0.979 for the line is very much close to the unity.

4. Conclusion

An ANN approach was used to delve into the complicated interactions between the process inputs and outputs for the removal of chromium (VI) from wastewater solution applying adsorption. The results offer an insight into the dependence of adsorption efficiency and adsorption capacity of the treatment process on pH of the wastewater, batch time, initial chromium (VI) concentration and activated carbon dosage. The most popular FF and BP algorithms were used to model the neural networks. A three-layered neural network, with different transfer functions namely "tansig", "satlin" and "poslin" at the hidden layer and "purelin" transfer function at the output layer, was used. The optimal neuron number is found to be in range of 8–11. Six backpropagation algorithms were compared to select the best-fitting backpropagation algorithms for the gathered data. This study shows that all algorithms and transfer functions are not suitable for this process. BFGS quasi-Newton backpropagation algorithm gave the most satisfactory results for adsorption efficiency while resilient backpropagation and BFGS quasi-Newton backpropagation algorithm were found to be the most suitable for adsorption capacity. The best combination of training algorithm and transfer function for adsorption efficiency was found to be trainrp and poslin, whereas poslin produced simulated results within 10% deviation during test and validation for adsorption capacity. The results presented in this paper confirm that the developed ANN model is equipped to be used in simulation work for design and development of automated effluent treatment plant for removal of chromium (VI). The simulated and experimental findings must have minimum deviation to a greater extent otherwise the targeted water quality could not be achieved. The formulated model can predict adsorption efficiency and adsorption capacity significantly and become successful for efficient run of an automated process. The model simulated in this work can further be implemented for performance investigation of chromium (VI) wastewater treatment over a broad spectrum of operating conditions.

Acknowledgements

Authors express their gratitude to all the lab members at Physical Chemistry, Pulping and Bleaching Division, Central Pulp and Paper Research Institute, Himmat Nagar, Saharanpur 247001, Uttarpradesh, India; Department of Chemical Engineering, Indian School of Mines, Dhanbad 826004, Jharkhand, India and Department of Chemical Engineering, Jadavpur University, Kolkata 700032, West Bengal, India for their cordial help and support during this work.

References

[1] K.Z. Setshedi, M. Bhaumik, S. Songwane, M.S. Onyango, A. Maity, Exfoliated polypyrrole-organically modified montmorillonite clay nanocomposite as a potential adsorbent for Cr(VI) removal, Chem. Eng. J. 222 (2013) 186–197.

[2] K.Y. Foo, B.H. Hameed, Insights into the modeling of adsorption isotherm systems, Chem. Eng. J. 156 (2010) 2–10.

[3] D. Aguado, J. Ribes, T. Montoya, J. Ferrer, A. Seco, A methodology for sequencing batch reactor identification with artificial neural networks: A case study, Comput. Chem. Eng. 33 (2009) 465–472.

[4] K. Anupam, S. Dutta, C. Bhattacharjee, S. Datta, Optimisation of adsorption efficiency for reactive red 198 removal from wastewater over TiO_2 using response surface methodology, Can. J. Chem. Eng. 89(5) (2011) 1274–1280.

[5] C.W. Baxter, S.J. Stanley, Q. Zhang, D.W. Smith, Developing artificial neural network models of water treatment processes: A guide for utilities, J. Environ. Eng. Sci. 1 (2002) 201–211.

[6] M.M. Hamed, M.G. Khalafallah, E.A. Hassanien, Prediction of wastewater treatment plant performance using artificial neural networks, Environ. Modell. Softw. 19(10) (2004) 919–928.

[7] B.V. Babu, V. Ramakrishna, K.K. Chakravarthy, Artificial neural networks for modeling of adsorption (2008). Accessed 25 June, 2011, doi: 10.1.1.110.1612. Available from: http://citeseerx.ist.psu.edu/viewdoc/summary.

[8] Y. Zhang, J. Xu, Z. Yuan, H. Xu, Q. Yu, Artificial neural network-genetic algorithm based optimization for the immobilization of cellulase on the smart polymer Eudragit L-100, Bioresour. Technol. 101 (2010) 3153–3158.

[9] A.B. Chelani, C.V.C. Rao, K.M. Phadke, M.Z. Hasan, Prediction of sulphur dioxide concentration using artificial neural networks, Environ. Modell. Softw. 17 (2002) 161–168.

[10] B.V. Babu, V. Ramakrishna, Applicability of regression technique for physical modeling: A case study on adsorption in wastewater treatment, Proceedings of International Symposium & 55th Annual Session of IIChE (CHEMCON-2002), Osmania Univeristy, Hyderabad, India, 2002.

[11] X. Du, Q. Yuan, J. Zhao, Y. Li, Comparison of general rate model with a new model—Artificial neural network model in describing chromatographic kinetics of solanesol adsorption in packed column by macroporous resins, J. Chromatogr. A 1145 (2007) 165–174.

[12] W. Gao, S. Engell, Estimation of general nonlinear adsorption isotherms from chromatograms, Comput. Chem. Eng. 29 (2005) 2242–2255.

[13] P.C. Nayak, Y.R.S. Rao, K.P. Sudheer, Groundwater level forecasting in a shallow aquifer using artificial neural network approach, Water Resour. Manage. 20 (2006) 77–90.

[14] K. Pramanik, Use of ANN for predication of cell mass and ethanol concentration in batch fermentation using *Saccbaromyces cerevisiae* yeast, J. Inst. Eng. (India) 85 (2004) 31–35.

[15] S. Lingireddy, G.M. Brion, Artificial Neural Networks in Water Supply Engineering, ASCE Publications, Reston, VA, 2005.

[16] C.M. Zealand, D.H. Burn, S.P. Simonovic, Short term streamflow forecasting using artificial neural networks, J. Hydrol. 214 (1999) 32–48.

[17] R. Hecht-Nielsen, Kolmogorov's mapping neural network existence theorem, Proceedings of the First IEEE International Joint Conference on Neural Networks, Institute of Electrical and Electronic Engineering, San Diego, CA, 1987.

[18] H.R. Maier, G.C. Dandy, Neural networks for the prediction and forecasting of water resources variables: A review of modelling issues and applications, Environ. Modell. Softw. 15(1) (2000) 101–124.

[19] M. Alp, H.K. Cigizoglu, Suspended sediment load simulation by two artificial neural network methods using hydrometeorological data, Environ. Modell. Softw. 22 (2007) 2–13.

[20] S. Birikundavyi, R. Labib, H.T. Trung, J. Rousselle, Performance of neural networks in daily streamflow forecasting, J. Hydrol. Eng. 7(5) (2002) 392–398.

[21] H.K. Cigizoglu, Incorporation of ARMA models into flow forecasting by artificial neural networks, Environmetrics 14(4) (2003) 417–427.

[22] D.E. Rummelhart, G.E. Hinton, R.J. Wiliams, Learning internal representations by error propagation, Report 8506, Institute for Cognitive Science, University of California, San Diego, CA, 1985.

[23] D. Mohan, C.U. Pittman Jr., Activated carbons and low cost adsorbents for remediation of tri- and hexavalent chromium from water, J. Hazard. Mater. 137 (2006) 762–811.

[24] K. Anupam, S. Dutta, C. Bhattacharjee, S. Datta, Adsorptive removal of chromium (VI) from aqueous solution over powdered activated carbon: Optimisation through response surface methodology, Chem. Eng. J. 173(1) (2011) 135–143.

[25] N. Zhao, N. Wei, J. Li, Z. Qiao, J. Cui, F. He, Surface properties of chemically modified activated carbons for adsorption rate of Cr (VI), Chem. Eng. J. 115 (2005) 133–138.

[26] G. Jing, Z. Zhou, L. Song, M. Dong, Ultrasound enhanced adsorption and desorption of chromium (VI) on activated carbon and polymeric resin, Desalination 279 (2011) 423–427.

[27] L.S. de Lima, M.D.M. Araujo, S.P. Quináia, D.W. Migliorine, J.R. Garcia, Adsorption modeling of Cr, Cd and Cu on activated carbon of different origins by using fractional factorial design, Chem. Eng. J. 166 (2011) 881–889.

[28] O. Ahmed, M. Nordin, S. Sulaiman, W. Fatimah, Study of genetic algorithm to fully-automate the design and training of artificial neural network, Int. J. Comput. Sci. Network Secur. 9(1) (2009) 217–226.

[29] H.R. Godini, M. Ghadrdan, M.R. Omidkhah, S.S. Madaeni, Part II: Prediction of the dialysis process performance using Artificial Neural Network (ANN), Desalination 265 (2011) 11–21.

[30] S. Lawrence, C.L. Giles, A.C. Tsoi, What size neural network gives optimal generalization? Convergence properties of backpropagation, Technical Report Umiacs-Tr-96-22 and CS-TR-3617, Institute for Advanced Computer Studies, University of Maryland, College Park, MD, 1996.

[31] K.V. Kumar, K. Porkodi, Modelling the solid–liquid adsorption processes using artificial neural networks trained by pseudo second order kinetics, Chem. Eng. J. 148(1) (2009) 20–25.
[32] H.R. Maier, N. Morgan, C.W.K. Chow, Use of artificial neural networks for predicting optimal alum doses and treated water quality parameters, Environ. Modell. Softw. 19 (2004) 485–494.
[33] K. Hornik, M. Stinchcombe, H. White, Multilayer feedforward networks are universal approximators, Neural Networks 2 (1989) 359–366.
[34] S. Dutta, S.A. Parsons, C. Bhattacharjee, S. Bandhyopadhyay, S. Datta, Development of an artificial neural network model for adsorption and photocatalysis of reactive dye on TiO_2 surface, Expert Syst. Appl. 37 (2010) 8634–8638.