Modeling of Removal of Chromium (VI) from Aqueous Solutions Using Artificial Neural Network

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ABSTRACT: *There is a need for knowledge, experience, laboratory, materials, and time to conduct chemical experiments. The results depend on the process and are also quite costly. For economic and rapid results, chemical processes can be modeled by utilizing data obtained in the past. In this paper, an artificial neural network model is proposed for predicting the removal efficiency of Cr (VI) from aqueous solutions with Amberlite IRA-96 resin, as being independent of chemical processes. Multiple linear regression, linear and quadratic particle swarm optimization are also used to compare prediction success. A total of 34 experimental data were used for training and validation of the model. pH, amount of resin, contact time, and concentration were used as input data. The removal efficiency is considered as output data for each model. The statistical methods of root-mean-square error, mean absolute percentage error, variance absolute relative error, and the coefficient of determination were used to evaluate the performance of the developed models. The system has been analyzed using a feature selection method to assess the influence of input parameters on the sorption efficiency. The most significant factor was found in pH. The obtained results show that the proposed ANN model is more reliable than the other models for estimating removal efficiency.*

KEYWORDS: *Artificial neural network; Multilinear regression; Particle swarm optimization; Cr(VI) removal, Modeling.*

INTRODUCTION

There is a need for knowledge, experience, laboratory, materials, and time to conduct chemical experiments. The results depend on the process and are also quite costly. For economic and rapid results, chemical processes can be modeled by utilizing data obtained in the past. It may make an unknown goal simple and clear by modeling. It also helps to analyze what happens during the process and confirm the results. Thus, there were conducted modeling studies for discovering many scientific relations in the past and recent years. Some of these studies are

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the river flow modeling [1], the precipitation-runoff modeling [2], the daily rainfall-runoff modeling [3], the tomato drying modeling [4], the hydrological modeling [5], the thermal conductivity modeling [6, 7], the modeling of the chemical biosorption and adsorption [8, 9] and modeling business failure [10]. Selecting the appropriate procedures for setting models is the main factor for making a right prediction [11]. There are a lot of modeling methods. Some of them are the artificial neural networks, the support vector machine, the genetic algorithm, the decision trees, the k-nearest neighbor algorithm and the Particle Swarm Optimization (PSO) algorithm. Artificial neural networks introduced by *McCulloch* and *Pitts* [12] have been used for prediction in many scientific studies. *Yetilmezsoy* and *Demirel* [13] developed an Artificial Neural Network (ANN) model to predict the removal efficiency of pistachio shells for Pb(II) ions from aqueous solution. The results of the studies showed that the modeling ability of ANN is better than Multi Linear Regression (MLR) by the low coefficient of MSE and high coefficient of R^2. *Fanaie et al.* [14] tried to predict the removal efficiency of p-chlorophenol with the help of activated sludge dried from aqueous solutions by ANN and Response Surface Methodology (RSM). In their study, they showed that the estimates by ANN are much closer to the actual values than the estimates by RSM. *Babaei et al* [15] conducted experiments for removal of methylene blue dye from aqueous solution in a particle system by activated spent tea which they had prepared and characterized by using different techniques (such as Brunauer-Emmett-Teller, Fourier transfer infrared and Scanning electron microscope). Experimental results have revealed that the Artificial Neural Network (ANN) based analysis is the most effective parameter for adsorbed dose and time of methylene blue adsorption.

Heavy metals are the major pollutants of marine, underground, industrial and even treated wastewaters [16, 17]. Some are very toxic even at low concentrations. Chromium, the more widely used one among these heavy metals, can be found in pigments and paints, leather tanning, fungicides, electroplating, cement, steel, ceramics and glass industries [18, 19]. The presence of Cr (VI) ions in wastewater from these industries has become a major concern today due to harmful effects on health and the environment [20-24].

Cr (VI) has a high health risk since it is dangerous for health because chromium in aqueous solutions can be absorbed by marine species easily and thus it may run into the human via food chain directly. For the last decade, one of the common applications for the removal of heavy metals present in the industrial waste water is ion exchange. Chelating resins are often used as ion exchange materials because their ligands can selectively bind to certain metallic ions [25].

One of these resins which is commercially provided is Amberlite IRA-96. The data from this study are extracted from the experimental studies relevant to removal efficiency of Cr (VI) ions from aqueous solutions by Amberlite IRA-96 under the effects of different parameters [25].

In this paper, an artificial neural network model is proposed for predicting the removal efficiency of Cr (VI) from aqueous solutions with Amberlite IRA-96 resin, as being independent of chemical processes. The artificial neural network is a data processing paradigm inspired by the biological nervous system such as the human brain. Multiple Linear Regression (MLR), linear and quadratic Particle Swarm Optimization (PSO) are also used to compare prediction success. Multiple linear regression analysis is one of the most commonly used modeling techniques in environmental research studies [26-29]. Multiple regression analysis is used to determine the existence of a cause and effect relationship between variables and to provide estimations or make predictions on the topic by using this relationship. The Particle Swarm Optimization (PSO) algorithm that was developed by *James Kennedy* and *Russell Eberhart* in 1995 is inspired by collective behavior of a bird swarm. It has been widely used to solve the optimization problems in various fields such as composite material, geotechnical engineering and synchronous motor design. A total of 34 experimental data were used for training and validation of the models. pH, amount of resin, contact time and concentration were used as input data. The removal efficiency is considered as output data for each model.

The main contributions of this article are that (i) the data used in the experiments were modeled by four different methods for the first time, (ii) additionally it was shown that chemical processes can be more economical (iii) and the optimum results may be achieved without any experiment.

EXPERIMENTAL SECTION

The removal of Cr (VI) by Amberlite IRA-96 resin

Cr (VI) metal solution was prepared as 200 ppm of $K_2Cr_2O_7$ (Merck, German) salt stock solution for the sorption studies. All metal solutions to be used later were prepared by diluting this stock solution with deionized water. Removal studies of Cr (VI) ions with commercially purchased Amberlite IRA-96 resin (Rohm & Haas, USA) were carried out as discrete experiments. The Cr (VI) ion removal studies conducted by commercially purchased Amberlite IRA-96 resin (Rohm & Haas, USA) were performed as discrete experiments. During the study, the effect of the various parameters such as pH, amount of resin, contact duration and initial metal concentration on the Cr (VI) removal was examined. During the experiments performed for determining the amount of resin, amount of Amberlite IRA-96 was changed between 0.01 and 0.1 g, and added to 25 mL of 50 ppm Cr (VI) solution and later the optimum resin amount was determined for maximum removal to be used for further experiments. At next step, the removal efficiency was observed at various time intervals between 5 and 240 minutes and the optimum contact time was determined. Thereafter, the optimum pH value was determined for maximum removal by changing the pH value of metal solution between 2.0 and 7.0. For adjusting the pH values of solutions, 0.1 M HCL (Sigma-Aldrich, German) and 0.1 M NaOH (Sigma-Aldrich, German) solutions were used. At the last step, the initial Cr (VI) solution concentration was prepared as changing the concentration between 10 and 100 ppm by diluting from stock solution and capacity values were calculated by Langmuir and Freundlich isotherm models.

ANN Model

The artificial neural network is a data processing paradigm inspired by the biological nervous system such as the human brain. The key element of this paradigm is the structure of the computing system [26]. A high number of connections are made between processing elements to solve certain problems of concern. Artificial neural networks learn with examples, similar to how people learn. An artificial neural network is shaped for precise application, such as data classification within a learning process or sample recognition. Learning requires rules being valid for biological nerves for connections that exist between the nerves.

The NNTool of the Matlab software platform was used for prediction of removal efficiency. ANN network consists of three layers that are shown in Fig. 1. They are named as input layer, hidden layer and output layer.

Input Layer: pH, adsorbent dosage, contact time and concentration were used as input variables to predict the removal efficiency of Amberlite IRA-96 for the removal of Cr (VI) ions in aqueous solutions.

Hidden Layer: Levenberg Marquard learning algorithm was used for this layer. For predicting the optimum removal efficiency, some of the parameters were changed and some of them were kept as stable. The parameters kept as stable were train function (trainlm), adaptive learning function (lerangdm) and transfer function (tansig). The number of hidden layers and number of neurons at hidden layers were changed for 16 different architectures to achieve better performance. As hidden layer, single layer and two layers were used. They were trained by 1, 3, 5, 7, 9, 11, 13 and 15 hidden neurons. Thereafter the trained model was used for prediction of the testing group (data used for simulation). In order to avoid numerical overflows, very large or small input and output data were normalized between 0.1 and 0.9 by the following formula:

$$y = 0.8\frac{(x_i - x_{min})}{x_{max} - x_{min}} + 0.1 \quad (1)$$

Output Layer: Removal efficiency of Amberlite IRA-96 was used as output variables.

MLR model

Multiple linear regression analysis is one of the most commonly used modeling techniques in environmental research studies. Multiple regression analysis is used to determine the existence of a cause and effect relationship between variables and to provide estimations or make predictions on the topic by using this relationship. A multiple linear regression model is stated as follows:

$$y = a_0 + a_1x_1 + a_2x_2 + \cdots a_nx_n + \varepsilon \quad (2)$$

In Equation (2), y is the dependent variable, x_1, x_2, …, x_n are independent variables, ε is the environmental error term, a_0 is the constant term and a_1, a_2, …, a_n are regression coefficients.

MLR analysis can be used for numerous purposes, one of which is for determining the effects of certain

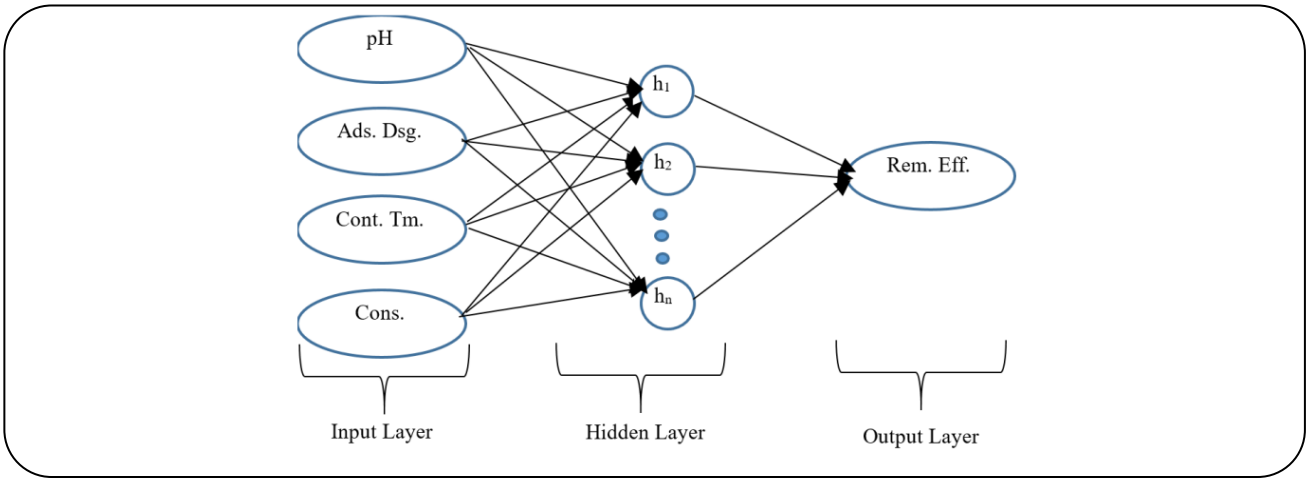

Fig. 1: Structure of ANN.

variables such as adsorbent dosage and pH in adsorption studies. In the present study, SPSS 15 statistics software was used for MLR analyses.

Particle swarm optimization algorithm

The Particle Swarm Optimization (PSO) algorithm that was developed by James Kennedy and Russell Eberhart in 1995 [30] is inspired by collective behavior of a bird swarm. It has been widely used to solve the optimization problems in various fields such as composite material [31], geotechnical engineering [32] and synchronous motor design [33]. The advantages of PSO are that it has only few parameters that need to be controlled and its implementation is very simple and easy.

PSO starts with a population randomly generated in a search space. Each particle in the population has two vectors: a velocity vector and a position vector. To discover the optimal solution, each particle changes its searching direction according to its personal best position (*pbest*) and global best position (*gbest*) obtained by the swarm so far. The velocity and the position of each particle are updated according to the Eqs. (3) and (4).

$$V_i^d = wV_i^d + c_1 rl_i^d \times \left(pbest_i^d - X_i^d\right) + c_2 \times r2_i^d \times \left(gbest^d - X_i^d\right) \quad (3)$$

$$X_i^d = X_i^d + V_i^d \quad (4)$$

Where i is the particle's index used as a particle identifier. V_{id} and X_{id} are the velocity and the position of the particle i in the dth dimension, respectively. c_1 is the acceleration coefficient for the cognitive component and c_2 is the acceleration coefficient for the social component. r_1 and r_2 are the stochastic components of the algorithm. They are randomly selected between 0 and 1. The constant w is called inertia weight and an important parameter in PSO. It plays the role to balance between the global search ability and local search ability [34]. The inertia weight w is updated according to the Eq. (5) during the optimization process.

$$w(t) = w_{max} - t\left(w_{max} - w_{min}\right)/T \quad (5)$$

Where w_{max} and w_{min} are the maximum and minimum inertia weights and usually set to 0.9 and 0.2, respectively [35]. t is the actual iteration number and T is the maximum number of iteration cycles.

The flowchart of the PSO is shown in Fig. 2 and the step by step procedure of the PSO algorithm is given as follows:

1. Initialize: The parameters of PSO are initialized and the population is randomly generated.

2. Update inertia weight: the inertia weight w is updated according to Equation (5).

3. Evaluation: The fitness value of each particle is evaluated.

4. Find *pbest*: If the fitness value of the particle i is better than the *pbest* of the particle i, the current fitness value is set as the new best of the particle i.

5. Find *gbest*: If any *pbest* is better than the *gbest*, *gbest* is set to this value.

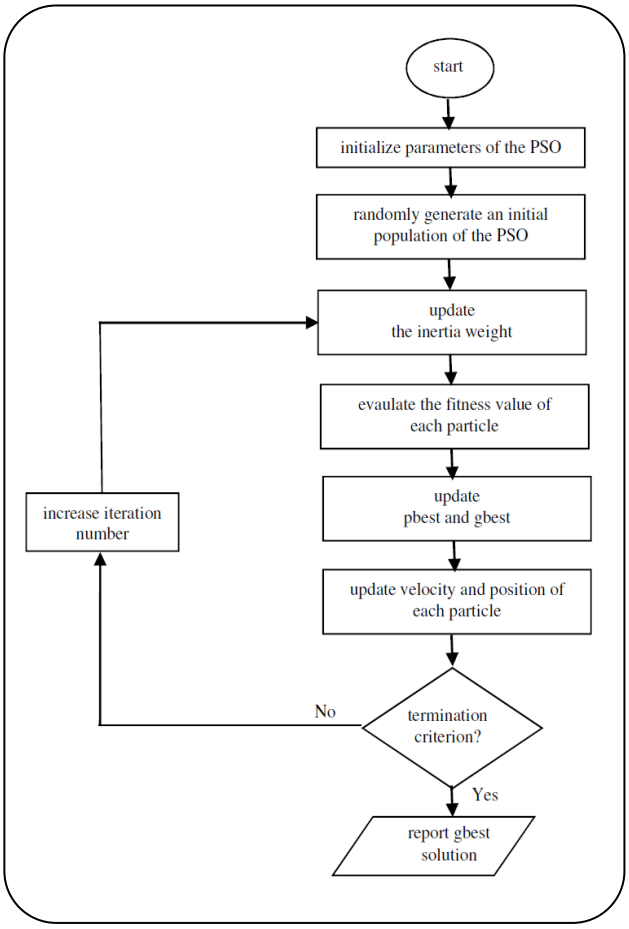

Fig. 2: The flowchart of the PSO algorithm.

6. Update velocity and position: The velocity of each particle is updated according to Equation (3), and the particle moves to the next position according to Equation (4).

7. Termination: If the stopping criterion is met, the algorithm will be stopped; otherwise it will be returned to step 2.

Performance Metrics

Also output performances of the models developed by different methods (ANN, MLR and PSO) were evaluated. Root Mean Square Error (RMSE), mean absolute percentage error (MAPE), variance absolute relative error (VARE) and the coefficient of determination (R^2) were found as evaluation criteria by the below formulas.

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_1^n \left(X_e - X_p\right)^2} \tag{6}$$

$$\mathrm{MAPE} = \frac{100}{n}\sum_1^n \left|\frac{x_e - x_p}{x_e}\right| \tag{7}$$

$$\mathrm{VARE} = \frac{1}{n}\left[\sum_1^n \left(\left|\frac{x_e - x_p}{x_e}\right| - \mathrm{mean}\left|\frac{x_e - x_p}{x_e}\right|\right)^2\right] \tag{8}$$

$$R^2 = 1` - \frac{\sum_1^n \left(x_p - x_e\right)\sum_1^n \left(x_p - x_e\right)^2}{\sum_1^n \left(x_e - \bar{x}\right)^2} \tag{9}$$

Where n represents the number of data sets, x_p and x_e represent the predicted and measured values, respectively. For a good model, the value of R^2 should be close to 1 while the values of RMSE, VARE and MAPE should be close to 0.

Sensitivity Analysis

In sensitivity analysis, feature selection model is constructed when the effects of the input parameters affecting the result are determined and the ineffective ones are eliminated. Proper selection of features is important for the inductive learner to improve learning speed, generalization capacity, reduce the size of the network, or model simplicity. In addition, working with fewer features also has other benefits such as reduced cost of measurement and better understanding of the problem area. Sensitivity analysis or feature selection was carried out to define the gradation efficiency of parameters using WEKA 3.8.2 data mining software.

RESULTS AND DISCUSSION

Prediction of removal efficiency

In this study, a simple ANN model was suggested to predict the removal efficiency of Amberlite IRA-96 for Cr (VI) ions in aqueous solution. MLR, linear and quadratic PSO models were developed to evaluate the success of the model. While the parameters of pH, amount of resin, contact time and concentration were considered as input data of the model, the removal efficiency was defined as output data. There showed intervals incident to data set used for the models and statistical analysis of data in Table 1.

Prediction of removal efficiency by ANN

Thirty-four experiment data were divided into 3 groups such as 70% training, 15% verification and 15% testing, to develop the ANN model. 16 different ANN architectures were tested for prediction of the best removal efficiency. The details relevant to the architectures were shown in Table 2.

Table 1: Ranges of data set and their statistics.

Parameters	Data Statistic		
	Ranges	Mean ± S.D.	Unit
Input Data			
pH	1.50 - 7.5	2.29 ± 1.75	
Ads. Dosage	25.00 - 100.0	32.89 ± 20.50	mg
Contact Time	30.00 - 180.0	74.21 ± 36.56	Min
Concentration	10.40 - 41.6	13.68 ± 8.52	ppm
Output Data			
Rem. Effic.	13.60 - 83.80	63.54 ± 25.29	%

Table 2: ANN parameters.

Parameters	Features
Network Type	Feed-forward
train func.	trainlm
adap.learnin func.	learngdm
hidden layer	1-2
neurons	1-3-5-7-9-11-13-15
layer 1 transfer func.	tansig
layer 2 transfer func.	logsig

In this study, the results of the developed ANN models using single hidden layer is not satisfactory. Therefore, the optimal topology for developed ANN model is the architecture having 2 hidden layers and 11 neurons (4-11-11-1). Each model was run for 500 epochs for training of the model by using Matlab NNTool. As a result, the R values for training, verification and testing were found to be 0.90, 0.91 and 0.87, respectively as seen in Fig. 3.

And RMSE values were found as 11.14 and 43.24. R^2, MAPE, RMSE and VARE values relevant to simulating data were found as 0.73, 6.81, 6.57 and 0.005, respectively. Our model predicts with 73% accuracy according to R^2, but having 6% error ratio according to MAPE. Table 3 consists of the results of experiments and prediction values relevant to ANN and the other models.

The actual values and the predicted values of the optimum ANN model are presented in Fig. 4. According to Fig. 4, it shows that the acceptability between predictions of ANN and actual values is very suitable.

Prediction of Removal Efficiency by MLR

The effects of experimental clauses were also modeled by MLR analysis. The equation incident to removal efficiency was formed by empirical data. SPSS 15.0 statistics program was used for the equation. The developed regression equation:

$$Y_{pre} = 0.094X_1 - 5.598X_2 - 0.407X_3 + 282.528X_4 + 94.577 \quad (10)$$

where the parameters X_1, X_2, X_3 and X_4 indicate the pH, resin amount, contact time and concentration, respectively.

The prediction values were calculated by using Equation (10). The related results were shown in Table 3.

Table 3: Models results of experiments and prediction values.

Observed Value	Predicted by ANN	Predicted by MLR	Predicted by L-PSO	Predicted by Q-PSO
72.117	72.264	70.811	70.806	79.756
60.237	72.256	59.615	59.610	61.707
91.793	85.737	76.357	76.351	77.770
88.994	94.881	97.734	97.737	96.094
90.834	91.461	87.647	87.646	96.470

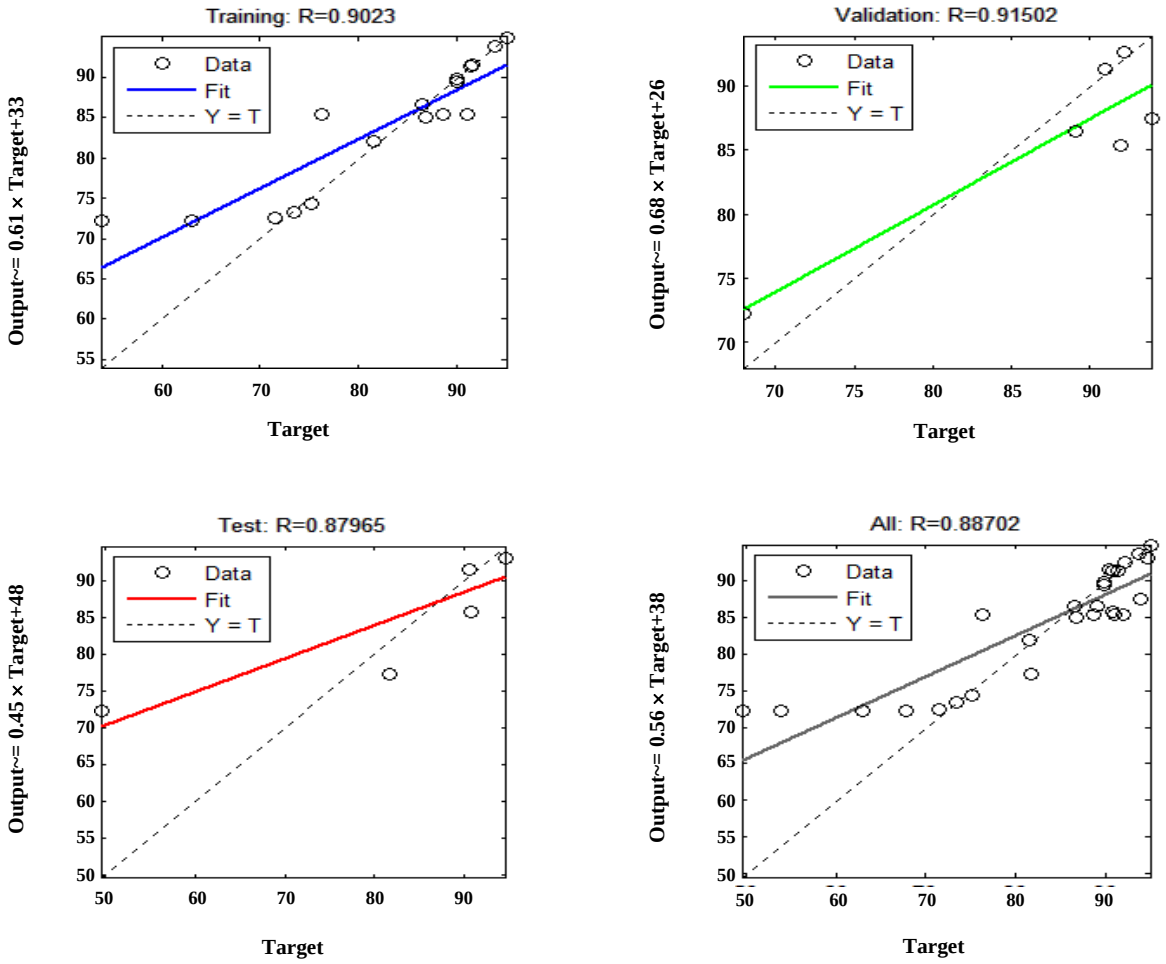

Fig. 3: Training regression result by ANN.

R^2, MAPE, RMSE and VARE values related with the data between the prediction for adsorption processes and results of the experiments are found as 0.59, 6.59, 8.08 and 0.003, respectively. It is shown that the ratio of MLR prediction is about 60%.

As examining R^2 and MAPE which are the performance criteria of the model produced by MLR, it is realized that MLR does not obtain a better result than ANN. A comparison is presented between prediction and simulated data belonged to MLR in Fig. 5.

Prediction of removal efficiency by PSO

In this section, the prediction of removal efficiency is modeled by using linear form in Equation (11) and

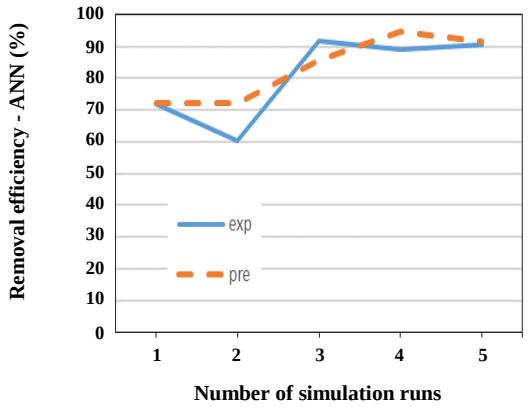

Fig. 4: Experimental values and predicted values for removal efficiency by ANN.

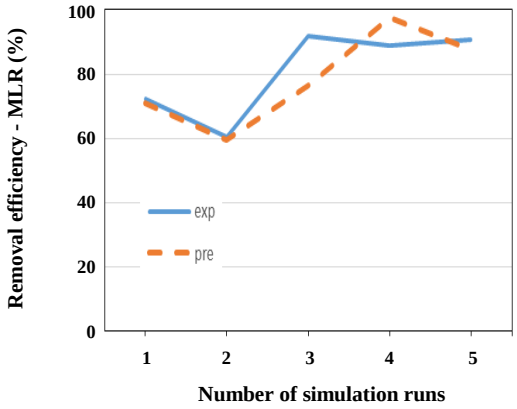

Fig. 5: Experimental values and predicted values for removal efficiency by MLR.

quadratic form in Equation (12). Four variables (pH, resin amount, contact time and concentration) were used in the model to predict the removal efficiency.

$$E_{linear} = w_1X_1 + w_2X_2 + w_3X_3 + w_4X_4 + w_5 \quad (11)$$

$$E_{quadratic} = w_1X_1 + w_2X_2 + w_3X_3 + w_4X_4 + w_5X_1X_2 + w_6X_1X_3 + w_7X_1X_4 + w_8X_2X_3 + w_9X_2X_4 + w_{10}X_3X_4 + w_{11}X_1^2 + w_{12}X_2^2 + w_{13}X_3^2 + w_{14}X_4^2 + w_{15} \quad (12)$$

Where the parameters X_1, X_2, X_3 and X_4 indicate the pH, resin amount, contact time and concentration, respectively. The coefficients of the model represent a possible food source position for the proposed method. The proposed model optimizes the coefficients (w_i) of the parameters (X_i). The aim is to find the fittest model to the input data. The fitness function of the algorithm is given as following:

$$\text{Min } f(X) = \sum_{k=1}^{N}\left(E_k^{experiment} - E_k^{predicted}\right)^2 \quad (13)$$

where N is the number of experiments. $E_k^{experiment}$ and $E_k^{predicted}$ are the actual value for kth experimental and the predicted value for kth experiment, respectively.

In the experiments, the parameters of PSO were set as follows: The linearly decreasing strategy [36] enhances the efficiency and performance of PSO. It is found experimentally that the inertia weight from 0.9 to 0.2 provides the excellent results. Hence, the inertia weight w dynamically decreases from 0.9 to 0.2 during the iterations. In literature, setting $c_1 = c_2 = 2$ has been proposed as a generally acceptable setting for most of problems and is widely used in practical applications of PSO [37]. Therefore, the acceleration coefficients c_1 and c_2 have a fixed value as 2 in the experiments. Population size is a critical parameter affecting the performance of population-based search techniques. Unfortunately, there are no universal rules to setting the size, and only experimental results give an idea of the behavior of the algorithms. It is preferable between 100 and 500 for the small-scale problems [38]. In the experiments, the population size and the maximum iteration number is 200 and 5000, respectively. The proposed model was tested 20 times and the best result was considered. According to the result of the experiments, the models shown in Equations (14) and (15) were developed.

$$E_{linear} = 0.09X_1 - 5.60X_2 - 0.41X_3 + 282.53X_4 + 94.58 \quad (14)$$

$$E_{quadratic} = -961.86X_1 - 114.52X_2 - 1075.50X_3 + 1064.76X_4 + 38.71X_1X_2 + 19.61X_1X_3 + 56.22X_1X_4 - 49.04X_2X_3 + 117.23X_2X_4 - 90.61X_3X_4 - 0.001X_1^2 - 1.49X_2^2 + 0.002X_3^2 - 3119.88X_4^2 + 53223.57 \quad (15)$$

L-PSO and Q-PSO were calculated by using the prediction values in Equation (14) and (15). L-PSO and Q-PSO predicted results were shown in Table 3. When R^2, MAPE, RMSE and VARE values belonged to L-PSO related with these results were found as 0.59, 6.60, 8.08 and 0.003, respectively. R^2, MAPE, RMSE and VARE values belonged to Q-PSO were found as 0.57, 8.49, 8.23

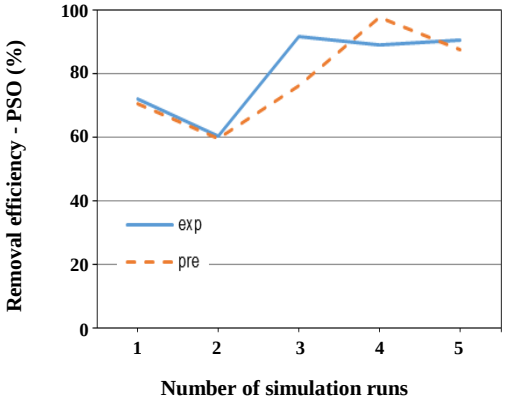

Fig. 6: Experimental values and predicted values for removal efficiency by L-PSO.

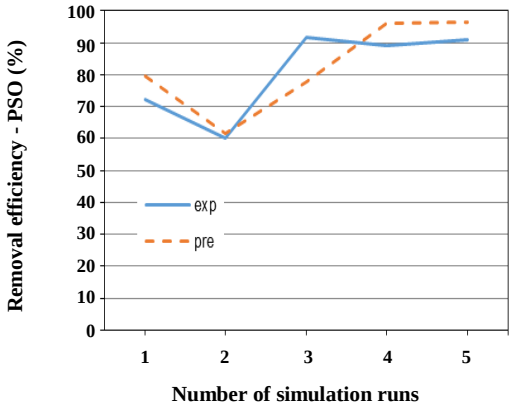

Fig. 7: Experimental values and predicted values for removal efficiency by Q-PSO.

and 0.001, respectively. Especially the prediction performance of L-PSO was found very close to MLR. However it was observed that both models (L-PSO and Q-PSO) could not reach the ANN prediction power.

Comparisons between prediction and simulated data belonged to L-PSO and Q-PSO are given in Figs. 6 and 7, respectively.

Evaluation of the Prediction Models

Four models were developed in this study to predict the removal efficiency of Amberlite IRA-96 resin for Cr (VI) removal being a heavy metal in aqueous solutions. These models are ANN, MLR, L-PSO and Q-PSO. 16 different ANN architectures were tested to find the optimum model among ANN models. The optimum topology among these architectures is the architecture which has 2 hidden layers with 11 neurons (4-11-11-1). The other details about the architecture were given in Table 2. Four different performance criteria (R^2, MAPE, RMSE and VARE) shown in Equations 2-5 were used to evaluate the optimum architecture. When considering R^2 among these criteria, it is realized that the model has 73% accuracy prediction ability. The model was found as having 6% error ratio as to MAPE. It was seen that the values of VARE and RMSE were close to 0. Three more models were developed as using multiple linear regressions, linear and quadratic particle swarm optimization methods to compare the prediction success of ANN as to these results. Q-PSO has a better performance than MLR and L-PSO among these 3 models. However, when comparing the performances of Q-PSO and ANN, it was found that ANN has better prediction ability. In [39], Response Surface Methodology (RSM) and Artificial Neural Network hybridized with Genetic Algorithm (ANN-GA) were used for modeling the removal efficiency of Cd(II) and optimizing the four removal process variables. Although both models were found to be effective in terms of predicting the removal efficiency of Cd(II), the ANN-GA model was found to be more accurate than the RSM model. In another study [40], sorption efficiency of cadmium was predicted by using adapted neural fuzzy model and a back propagation artificial neural network and it was found that adaptive neuro-fuzzy inference system proved to be more efficient in predicting Cd adsorption than a single layered feed forward artificial neural network. A single-layer Artificial Neural Network (ANN) model was used to predict the Sorption Efficiency of Leaf Powder (SILP) in [41] and the Levenberg–Marquardt algorithm (LMA) was found best of Back Propagation algorithms with a minimum Mean Squared Error (MSE). In [42], a four-layer fast artificial neural network was used and tested to model the sorption efficiency of Cd metal ions onto valonia tannin resin VTR. It was resulted that the applied technique of ANN has better adjusted the equilibrium data of the Cd adsorption when compared with the conventional isotherm models. As a result of the study performed in [43] where ANN was used for modeling the sorption of Cd ions by nanocellulose fibers, a single layer ANN model was developed. It was indicated that ANN provided reasonable predictive performance for training, cross validation and testing data sets. In [44],

Table 4: Comparison of the ANN, MLR and PSO models according to R^2, MAPE, RMSE and VARE.

Models	Performance criteria			
	R^2	MAPE	RMSE	VARE
ANN	0.73	6.81	6.57	0.005
MLR	0.59	6.59	8.08	0.003
L-PSO	0.59	6.60	8.08	0.003
Q-PSO	0.57	8.49	8.23	0.001

the adsorption process was modeled via A three layer feed forward Artificial Neural Network (ANN) with back propagation training algorithm. It was determined as a result of the study that the neural network model predicted values are found in close agreement with the batch experiment result with correlation coefficient (R) of 0.995 and Mean Squared Error (MSE) 0.0043975. In another study [45], a two-layer ANN model combined with back propagation was developed for the sorption efficiency of a biomaterial for the removal of Cd(II). As a result of this study, the Levenberg-Marquardt Algorithm (LMA) was applied, giving a minimum mean squared error (MSE) for training and cross validation at the ninth place of decimal.

Performance comparison between ANN and the other 3 models was summarized in Table 4.

It may be understood that ANN will be used as a more powerful model for prediction of removal efficiency. Comparison between prediction and experimental data belonged to ANN, MLR, L-PSO and Q-PSO was shown in Figs. 4-7 by utilizing Table 3.

Evaluation of the sensitive analysis

The software used for the sensitive analysis is WEKA data mining software. An attribute evaluator named "Correlation Attribute Eval" was used and the factors affecting sorption of the input parameters are determined according to ranked by importance. "Correlation Attribute Eval" evaluates an attribute value by measuring the correlation between it and the parameters that affect it. The results are shown in Table 5.

According to Table 5, the pH is the most effective parameter, while the effect of concentration seems to have least effect. The parameters in the order of pH > contact time > adsorbent dosage > concentration were found to be the most significant factors (Fig. 8).

Table 5: Input parameters and ranked attributes.

Input Parameter	Rate
pH	0.645
Adsorbent Dosage	0.372
Contact Time	0.398
Concentration	0.231

CONCLUSIONS

The main aim of this study is to develop a model which may predict the removal efficiency for Cr (VI) being one of the heavy metals existing in aqueous solutions. For this purpose, the models based on ANN, MLR and PSO were developed. pH, amount of resin, contact time and concentration were used as input data for models. The output data show the removal success of Cr (VI) in aqueous solutions. Thirty-four experimental data were utilized for developing the models. Some of the experimental data were used for simulation to evaluate the real performance of the models. The performances of simulation results were evaluated by R^2, MAPE, RMSE and VARE statistical methods. As to these results, when the highest R^2 (0.73) belongs to ANN model, R^2 values of the other models were between 0.57 and 0.59. Similarly when RMSE value of ANN model is 6.57, RMSE values of the other models were close to each other and they were about 8.15. In conclusion, it was determined that the prediction ability of ANN model is significantly higher than the other models. Additionally it was found that ANN is a powerful model for prediction of removal efficiency for removing heavy metal Cr (VI) existing in aqueous solutions. The system has been analyzed using feature selection method to assess the influence of input

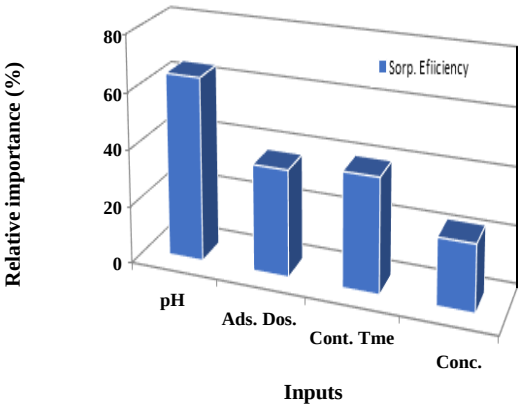

Fig. 8: Relative importance of inputs affecting the sorption efficiency.

parameters on the sorption efficiency. The most significant factor was found as pH.

As a further study, it is thought that using ANN method as a hybrid with the optimization algorithms like PSO will increase the prediction power and thus such a study is aimed.

Conflict of interest The authors declare that they have no conflict of interest.

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