Neural Network Modeling and Simulation of Sorption of Cd (II) Ions from Waste Water using Agricultural Waste

J. K. Arora and Shalini Srivastava

Abstract
A single-layer Artificial Neural Network (ANN) model was developed to predict the removal efficiency of Cd (II) ions from aqueous solution using *saraca indica* leaf powder (SILP). Batch experiments resulted into standardization of optimum conditions: biomass dosage (4.0 g), Cd (II) concentration (25 mg/l) volume (200 ml) at pH 6.5. A time of forty minutes was found sufficient to achieve the equilibrium. The ANN model was designed to predict sorption efficiency of SILP for target metal ion by combining back propagation (BP) with principal component analysis. A sigmoid axon was used as transfer function for input and output layers. 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.

Keywords: Neural Network Application; Artificial neural network; Biosorption; *SILP*; Cd (II) removal

1. Introduction

Heavy metal pollution of aqueous streams is a major environmental problem facing the modern world. Currently used water treatment technologies for Cd (II) involves chemical precipitation, evaporation, electro-chemical treatment, ion exchange [2]. However, these processes are economically non-feasible especially for the developing countries. Biosorption of heavy metals is one of the most promising and tangible alternatives to traditional methodologies. Biomaterials have gained much importance for decontamination of water which involves processes that reduce overall treatment cost through the application of wastes like bagasse pith, wood, saw dust and other agricultural wastes [3, 4].

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To achieve an optimum management for any control measure, the concept of modeling for an efficient operation and design should be developed. The mechanism of biosorption is highly complex and is difficult to model and simulate using conventional mathematical modeling. This is mainly due to interaction of more number of sorption process variables, and hence the resulting relationships are highly non linear. ANN utilizes interconnected mathematical neurons to form a network that can model complex functional relationship [5]. In recent years, ANN have been used as a powerful modeling tool in various processes such as membrane filtration, gas separation, ultra filtration, reverse osmosis etc. [6, 7].

In continuation of our work on biosorption of toxic metals using agricultural waste from waste water [8-11], the present paper describes the abatement of Cd (II) ions from aqueous system using *saraca indica* leaf powder (SILP). It also reports the applicability of a single layer ANN model using a back propagation (BP) algorithm to predict the removal efficiency of SILP for Cd (II) ions. Pursuing benchmark comparisons of BP algorithms, a study was conducted to determine the optimization study to determine the optimal network structure. Experimental data were initially distributed to three subsets; training, validation and testing. Finally, output obtained from the ANN modeling was compared with the experimental data. The present piece of work highlights the possibility of the prediction of sorption efficiency for the metal ions from waste water using SILP in the range of metal concentration with which lab experiments have not been conducted.

2. Materials and Methods

2.1. Biosorbent preparation

Leaves of *Saraca indica* Linn. were collected from the target plant. They were washed repeatedly with water to remove dust and soluble impurities, dried at 65 ^{o}C for 24 hours, crushed and finally sieved through (105μm) mesh copper sieves. *Saraca indica* leaf powder (SILP) was used as biosorbent.

2.2. Biosorption studies

Sorption studies using standard practices were carried out in batch experiments (triplicate) as a function of biomass dosage (2.0-6.0 g), contact time (10-60 min), volume of the test solution (100-300 ml), metal concentration (10-100 mg/l), particle size (105) and pH (4.5-8.5). The details of methodology have been described in our earlier publications. Percent metal uptake by the sorbent has been computed using the equation: % Sorption = Co – Ce / Co · 100, where Co and Ce were the initial and final concentration of metal ions in the solution.

2.3. Statistical analysis

Batch experiments were conducted in triplicates (N = 3) and data represent the mean values. Regression, correlation coefficients, standard deviations have been calculated using SPSS PC+TM statistical package.

2.4. Definition of the ANN model

Neural Network Toolbox Neuro Solution 5 ® mathematical software was used to predict the sorption efficiency. Ninety experimental sets were used to develop the ANN model. A single-layer ANN with sigmoid axon transfer function was used for input and output layers. The data gathered from batch experiments were divided into input matrix and desired matrix. The single layer sigmoid network represents functional relationship between inputs and output, provided sigmoid layer has enough neurons. Levenberg-Marquardt algorithm is fastest training algorithm for network of moderate size, therefore, used in the present study.

3. Results and discussions

3.1. Sorption Studies

Sorption studies led to the standardization of the optimum conditions as: Cd (II) concentration (25 mg/l), contact time (40 min) and volume (200 ml) at pH 6.5 for maximum Cd (II) removal (92.60%). The results indicate that the SILP has considerable potential to be used as biosorbent for metal removal from waste water. Studies, therefore, have been planned to predict the efficiency of SILP for the removal of Cd (II) using ANN model.

3.2. Optimization of the ANN structure

The prediction of removal efficiency of Cd (II) ions from aqueous system using SILP are made in the range of metal concentration with which experiments have not been conducted. A training set of ninety experimental data sets was selected to develop the model. ANN model based on single layer recurrent back propagation algorithm for the experimental data was applied to train the neural network. During training, the output vector is computed by a forward pass in which the input is propagated forward through the network to compute the output value of each unit. The output vector is then compared with the desired vector which resulted into error signal for each output unit. In order to minimize the error, appropriate adjustments were made for each of the weights of the network. After several such iterations, the network was trained to give the desired output for a given input vector. The optimum network structure was determined as single layer with 15 hidden neurons (1500 epochs) describing the dynamics of Cd (II) in effluent (Fig. 1) respectively.

The sigmoid axon was considered transfer function with 0.7 momentums. The performance of neural network simulation was evaluated in terms of mean squared error (MSE) criterion. The MSE for the training and cross validation data sets were found at the ninth place of decimal. The developed network model was examined for its ability to predict the response of experimental data not forming part of the training program. Fig.2 show the result obtained by the network simulation for both the training and cross validation data sets. The reduction in Cd (II) concentrations were precisely predicted for the training data sets. The development of the proposed ANN model is an effort towards the growing interest in applying ANN modeling technique to the area of biosorption of pollutants from water bodies [12-14].

3.3. Sensitivity analysis

A sensitivity analysis was conducted to determine the degree of effectiveness of variables. Performance of the groups of input vectors included biomass dosage, Cd (II) ion concentration, contact time and volume of test solution. Series of experiment resulted into the evaluation of the performance based on 60 % data for training, 20 % data for testing and 20 % data for cross validation at 1500 Epoch with 0.70000 momentums. The minimum MSE in the group of four variables determined for training and cross validation were as 0.001725798 and 0.001732187 respectively as shown in the Table 1. The effect of various experimental parameters was studied and compared with performance of ANN model based predictions.

3.4. Effect of metal concentration on the sorption efficiency

Fig. 3 represents the effect of metal concentration on the sorption behavior of Cd (II) on SILP in the range of metal concentration (10–100 mg/l). Sorption of Cd (II) on SILP increased with increasing concentration of the metal ion reaching to an optimal level (25 mg/l). Later,

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an increase in initial concentration decreased the percentage binding. These observations can be explained by the fact that at medium concentrations, the ratio of sorptive surface area to metal ions available is high and thus, there is a greater chance for metal removal [15]. The experimental data and ANN calculated outputs were compared and found that the ANN model shows a good performance on prediction of the experimental data.

3.5. Effect of biomass dosage on the sorption efficiency

Percent sorption increased with the increase of biomass dosage from 2.0 to 6.0 g. However, no significant increment in the sorption tendency was observed on further increasing the biomass dosage from 4.0 g onwards. This might be due to attainment of equilibrium between adsorbate and adsorbent. The perusal of experimental data and ANN outputs, as a function of biomass dosages (Fig. 4) depicted the performance of the model in good harmony with the experimental data.

3.6. Effect of initial volume on the sorption efficiency

The effect of volume on the percent sorption of Cd (II) on SILP was observed under similar experimental conditions in different set of volumes (100–300 ml). Maximum sorption was obtained in the volume (200 ml) of the test solution. It shows that the ratio of sorption surface of the SILP to total Cd (II) ions availability is optimum, exhibiting maximum percentage removal (92.60%). ANN model showed performance in resemblance with experimental data (Fig. 5).

3.7. Effect of contact time on the sorption efficiency

The effect of contact time on Cd (II) sorption on SILP was studied for duration of 10–60 minutes. The percent sorption metal ion gradually increased with time from 10 to 30 minutes, finally reaching the optimum value at 40 minutes. ANN model prediction was found in match with experimental data.

3.8. Effect of pH on sorption efficiency

The pH of a suspension is an important factor that can affect the percentage sorption of Cd (II) ion on SILP. The sorption efficiency increases, as the pH of the solution is increased from 4.5 to 8.5. The pH profile for Cd (II) sorption on seed powder shows that metal sorption is a function of pH, exhibiting maximum sorption at pH 6.5. Investigation on pH variation beyond 7.5 yielded an increase in sorption up to pH 8.5 which might be due to the precipitation carryover of Cd (II) ion which starts at pH 7.5. ANN model predictions were made at optimum pH 6.5.

4. Conclusion

The present piece of work demonstrates the successful removal of Cd (II) ions from the aqueous solutions using *Saraca indica* leaf powder (SILP) with maximum removal efficiency (92.60%). The single layer ANN modeling technique was applied to optimize this process. The Levenberg–Marquardt algorithm (LMA) was found best of BP algorithms with a minimum mean squared error (MSE) for training and cross validation as 0.001725798 and 0.001732187 respectively. Introduction of knowledge-based systems is efficient for scientific research of unstudied dependence among different by natural variables (physical, chemical, biological) for solving tasks of inferential measurement and process optimization without requiring a big amount of precise experimental data.

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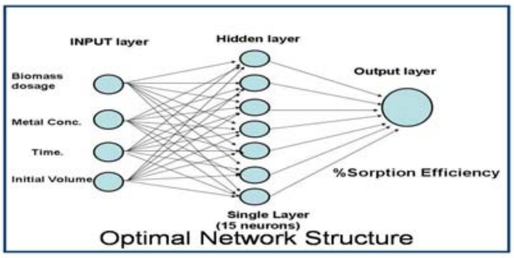

Figure 1. Single layer Optimum Neural Network structure for the prediction of the biosorption efficiency.

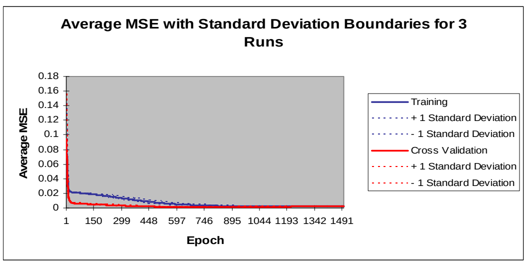

Figure 2. Graphical representation of MSE value with 1500 Epoch

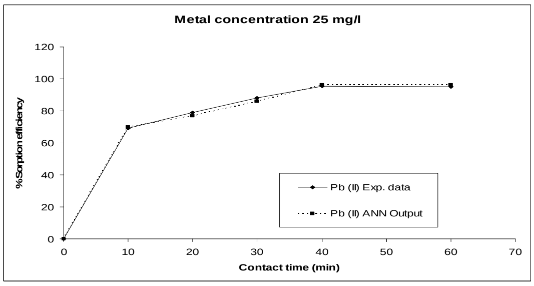

Figure 3. Agreement between ANN outputs and experimental data as a function of metal concentration 25 mg/l (biomass dosage = 4.0g, volume = 200ml and pH= 6.5).

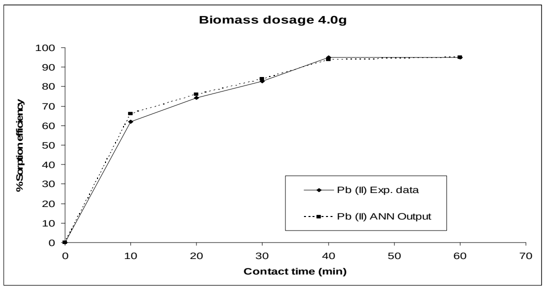

Figure 4. Agreement between ANN outputs and experimental data as a function of biomass dosage 4.0g (metal concentration = 25mg/l, volume = 200ml and pH= 6.5).

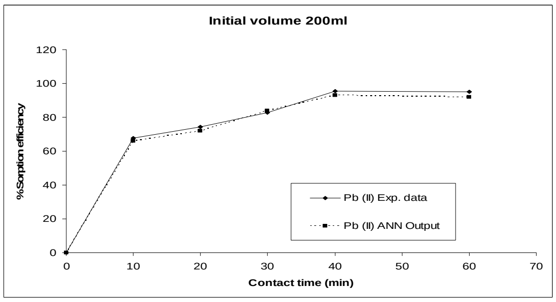

Figure 5. Agreement between ANN outputs and experimental data as a function of volume 200ml (metal concentration = 25mg/l, biomass dose = 4.0g and pH= 6.5).