Modeling of Electrodialysis Using Neural Network

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Abstract
In this paper, separation of lead ions with the aid of a laboratory scale electrodialysis (ED) cell was modeled using artificial neural network (ANN) technique. Separation percent (SP) of lead ions was predicted at various concentrations (100, 500, and 1000 ppm), temperatures (25, 40, and 60 °C), flow rates (0.07, 0.7, and 1.2 mL/s) and voltages (10, 20, and 30 V). An ANN structure with two hidden layers (4:5:4:1) was used for prediction. The modeling results showed that there is an excellent agreement between the experimental data and the predicted values, with mean absolute errors less than 1%. ANN modeling technique was found out to have many favorable features such as efficiency, generalization and simplicity, which make it an attractive choice for modeling of complex systems, such as wastewater treatment processes.

Keywords: Electrodialysis, Neural Network, Wastewater Treatment, Metal Ions

1. Introduction

Many industrial wastewaters produced by metal plating, metal finishing, mining, automotive, aerospace, battery and general chemical plants, often contain high concentration of heavy metals [1]. Lead is a highly toxic heavy metal. It impairs hemoglobin synthesis, particularly in children, and may cause neurological disorders. Wastes that include lead are found in paints, pipes, batteries and in some petrol types [2].

Membranes can also be used to obtain effluents without metallic contaminants. ED is an electro-membrane process for separation of ions across charged membranes, which has been widely used for production of drinking and process water from brackish water and seawater, treatment of industrial effluents, recovery of useful materials from effluents and salt production [18-20].

Artificial neural networks (ANNs) demonstrated to be an effective

The conventional heavy metal removal processes such as chemical precipitation [3] coagulation, complexing, solvent extraction [4-6], ion exchange [7,8], biosorption [9-13] and electro-membrane processes [14-16] and ion exchange/adsorption on solid surfaces [17] has some inherent shortcomings such as requiring a large area of land, a sludge dewatering facility, skillful operators, High capital and regeneration costs and multiple basin configurations [3].

predictive instrument for modeling the behavior of nonlinear dynamic systems, typical of several engineering applications. The interest of scientific and academic community towards the applications of ANNs to membrane technology is progressively increasing. In recent years, ANNs have been used as a powerful modeling tool in various membrane processes such as membrane filtration, microfiltration, ultrafiltration, nanofiltration, reverse osmosis, gas

separation, membrane bioreactors and Fuel Cells. But, no record for modeling of ED desalination by ANN was surprisingly found in the literature.
The objective of this paper is to develop a multi layer perceptron (MLP) neural network model in order to predict SP of lead ions during ED of wastewater.

2. Theory

The objective of a neural network is to compute output values from input values by some internal calculations. The basic component of a neural network is the neuron, also called "node". Figure 1 illustrates a single node of a neural network.
Inputs are represented by a_1, a_2 and a_n, and the output by O_j. The node manipulates these inputs to give a single output signal. The values w_{1j}, w_{2j}, and w_{nj}, are weight factors associated with the inputs to the node. Weights are adaptive coefficients within the network that determine the intensity of the input signal. Every input (a_1, a_2, …, a_n) is multiplied by its corresponding weight factor (w_{1j}, w_{2j}, …, w_{nj}), and the node uses summation of these weighted inputs (w_{1j} a_1, w_{2j} a_2, …, w_{nj} a_n) to perform further calculations. In the initial setup of a neural network, weight factors usually are chosen randomly according to a specified statistical distribution [21].
The other input to the node, b_j, is the node's internal threshold, also called bias. This is a randomly chosen value that governs the node's net input through the following equation:

$$u_i = \sum_{i=1}^{n}\left(w_{ij}a_i\right) - b_j \qquad (1)$$

Node's output is determined using a mathematical operation on the node's net input. This operation is called a transfer function. Sigmoid transfer function, which was applied in the present work, is as follows:

$$f(x) = \frac{1}{1+e^{-x}} \qquad 0 \le f(X) \le 1 \qquad (2)$$

The neuron's output, O_j, is found by performing one of these functions on the neuron's net input, u_j. Neural networks are made of several neurons that perform in parallel or in sequence [22].

3. Experimental

An analytical grade salt (99.9% lead nitrate supplied by Merck) and deionized water were used in all experiments to produce solutions with wastewater qualities. The ED cell was packed with a pair of cation and anion exchange membranes (CEM and AEM) and a pair of platinum electrodes (anode and cathode). Both electrodes were made of pure platinum. Area of each electrode was 4.2 × 4.2 mm^2. Thickness of dilution cell (center) was 4 mm and thickness of each concentrate cell (left and right) was 3 mm. Schematic view of the applied ED cell is presented in Figure 2. Lead nitrate solution is introduced into the three compartments. When a DC potential is applied between two electrodes, positively charged lead ions move toward the cathode, pass through the negatively charged CEM and are retained by the positively charged AEM. On the other hand, nitrate ions move toward the anode, pass through the AEM and are retained by the CEM. At the end, ion concentration increases in the side compartments with a simultaneous decrease of ion concentration in the middle compartments.
AR204SXR412 and CR67, MK111 anion and cation exchange membranes supplied by Arak petrochemical complex and made by Ionics incorporated were used in all experiments. Effective area of each membrane was 6 × 6.5 mm^2.
According to our previous studies [2,20,23], four parameters, each at three levels (temperature 25, 40 and 60 °C; concentration 100, 500 and 1000 ppm; flow rate 0.07, 0.7 and 1.2 mL/s; Voltage 10, 20 and 30 V) were investigated. SP

defined as follows was used as a criterion of the cell performance:

$$SP = \frac{C_0 - C}{C_0} \times 100 \quad (3)$$

Where, C_0 and C are feed and dilute concentrations, respectively. Concentration of cations (Pb^{2+}) only in the dilute compartment was measured with the aid of atomic absorption (Shimadzu, AA-670).
Totally 81 experimental data are collected and used for ANN modeling of ED for training/validation/testing subsets. In this work, feedforward multilayer neural network with two hidden layers was employed for modeling of ED. It was used to transform input data (concentration, temperature, flow rate and voltage) into a desired response (SP). Figure 3 illustrates the structure of the ANN used for modeling of ED.

4. Results and Discussion

The total 81 experimental data were randomly divided into three subsets of training, validation and testing for developing ANN model. Distribution of these data is shown in Figure 4. 50 training data were used to update the network weights and biases. In order to check the generality of network prediction and to prevent the data overfitting 21, validation data were applied. The rest of data was used to test the neural network.
The MLP networks were created in the neural network toolbox of Matlab with *newff* function. Performances of different training algorithms were studied for a specified network with four layers (1 input layer/ 2 hidden layer/ 1 output layer). Due to the convergence speed and the performance of network to find better solution, the Levenberg–Marquardt training method was selected as a proper training.
Another important factor in ANN design is the type of transfer functions. ANNs owe their non-linear capability to the use of non-linear transfer functions. Different transfer functions can be used for neurons in the different layers. Among different transfer functions available in Matlab, log sigmoid function was selected for all neurons due to its better prediction performance than other transfer functions. The log sigmoid function is bounded between 0 and 1, so the input and output data should be normalized to the same range as the transfer function used. In other words, the logarithmic sigmoid transfer function gives scaled outputs (SP) in this range (0 to 1).
Network structure has significant effects on the predicted results. The number of input and output nodes, as mentioned before, is equivalent to the number of input and output data, respectively (4 and 1 in this work). However, the optimal number of hidden layers and the optimal number of nodes in each layer, are case dependent and there is no straightforward method for determination of them. In this study, optimum structure was found to be 4:5:4:1 (2 hidden layers with 5 and 4 neurons in the first and second layer, respectively), as illustrated in Figure 4.
Another important factor that affects the performance of networks is selection of the initial weights. Typically, the weight factors are set randomly using either normal or Gaussian distribution. The wrong choice of initial weights can lead to the local minimum values and therefore bad performance of the networks. In order to prevent these phenomena, 20 runs were performed using different random values of initial weights and the best trained network was selected.
In Figure 5, the experimental results versus neural network predictions of the selected network (4:5:4:1) is plotted at the minimum MSE of validation data. According to this figure, excellent performance of the 4:5:4:1 network is confirmed.
The selected network was used to predict SP for different inputs in the domain of training data. In Figures 6-8, SP is plotted

versus operating parameters in 3D plots. As can be seen, increasing temperature, concentration and voltage increases SP values. It is obvious due to the fact that increasing temperature and concentration decreases the electrical resistance of solution, while increasing voltage increases the driving force. At higher flow rates, SP values decreases because the more flow rate means the less residence time, and thus, ions that are between the membranes do not have enough time to transfer through them. The generalization performances of 4:5:4:1 network, show no oscillations and this confirms an excellent prediction performance of ANN. ANN predictions can also be used for optimization purposes.

5. Conclusion

ANN was employed as an interesting method for modeling of ED; a wastewater treatment process. A multilayer network (FFNN-MLP), with two hidden layers (4:5:4:1), was applied to predict SP of Pb^{2+} ions in the dilute compartment of a laboratory scale ED cell. ANN successfully tracked the nonlinear behavior of SP versus temperature, voltage, concentration and flow rate with standard deviation not more than 1%. For almost all experiments, the ANN was confirmed to be an adequate interpolation tool, where good prediction was obtained. ANN is found out to be an efficient tool to model the complicated ion transfer mechanism in an electrical field.

References

[1] P. Canizares, A. Perez, R. Camarillo, Recovery of heavy metals by means of ultrafiltration with water-soluble polymers: calculation of design parameters, Desalination 144 (2002) 279-285

[2] T. Mohammadi, A. Razmi, M. Sadrzadeh, Effect of operating parameters on Pb^{2+} separation from wastewater using electrodialysis, Desalination 167 (2004) 379-385

[3] P. Zhou, J.C. Huang, A.W.F. Li and S. Wei, Heavy metal removal from wastewater in fluidized bed reactor, Water Research 33(8) (1999) 1918-1924

[4] S.R. E1-Hasani, S.M. AI-Dhaheri, M.S. EI-Maazawi and M.M. Kamal, Polarographic and voltammetric determination of some toxic heavy metal ions in the treated wastewater at Abu-Dhabi, UAE, Water Science and Technology 40(7) (1999) 67-74

[5] E. Rodryguez de San Miguel, J.C. Aguilar, M.T.J. Rodryguez and J. De Gyves, Solvent extraction of Ga (III), Cd (II), Fe (III), Zn (II), Cu (II), and Pb (II) with ADOGEN 364 dissolved in kerosene from 1-4 tool dmy3 HCI media, Hydrometallurgy 57 (2000) 151-165

[6] A.R.K. Dapaah, N. Takano and A. Ayame, Solvent extraction of Pb(II) from acid medium with zinc hexamamethylenedithiocarbamate followed by backextraction and subsequent determination by FAAS, Analytica Chimica Acta 386 (1999) 281-286

[7] V.J. Inglezakis, M.D. Loizidou and H.P. Grgorooulou, Equilibrium and kinetic ion exchange studies of Pb^{2+}, Cr^{3+}, Fe^{3+} and Cu^{2+} on natural clinoptilolite, Water Research 36(11) (2002) 2784-2792

[8] M.V. Mier, R.L.P. Callejas, R. Gehr, B.E.J. Cisneros and P.J.J. Alvarez, Heavy metal removal with Mexican clinoptilolite: Multi-component ionic exchange, Water Research 35(2) (2001) 373-378

[9] A. Vecchio, C. Finoli, D. Di Simine and V. Andreoni, Heavy metal biosorption by bacterial cells, Fresenius, Journal of Analytical Chemistry 361(4) (1998) 338-342

[10] M.L. Merroun, N. Ben Omar, M.T. Gonzalez Munoz and J.M. Arias, Removal of lead from aqueous solutions by *Myxococcus xanthus,* International Biodeterioration Biodegradation 37(3-4) (1996) 241

[11] M. Bustard and A.P. McHale, Biosorption of heavy metals by distillery-derived biomass, Bioprocess Engineering., 19(5) (1998) 351-353
[12] A.A. Pradhan and A.D. Levine, Microbial biosorption of copper and lead from aqueous systems, The Science of the Total Environment 170 (1995) 209-220
[13] J.M. Brady and J.M. Tobin, Binding of hard and soft metal ions to *Rhizopus arrhizus biomass*, Enzyme and Microbial Technology 17 (1995) 791-796
[14] V. Gopal, G.C. April and V.N. Schrodt, Selective lead ion recovery from multiple cation waste streams using the membrane-electrode process, Separation and Purification Technology 14 (1998) 85-93
[15] K. Basta, A. Aliane, A. Lounis, R. Sandeaux, J. Sandeaux and C. Gavach, Electroextraction of Pb^{2+} ions from dilute solutions by a process combining ion-exchange textiles and membranes, Desalination 120 (1998) 175-184
[16] R.S. Juang and S.W. Wang, Metal recovery and EDTA recycling from simulated washing effluents of metal contaminated soils, Water Research 34(15) (2001) 3795-3803
[17] G. Banerjee and S. Sarker, The role of salvinia rotundifolia in scavenging aquatic Pb(II) pollution: a case study, Bioprocess Engineering 17 (1997) 295-300
[18] W.S. Winston Ho, K.K. Sirkar, Membrane Handbook, Champan & Hall, 1992
[19] T. Mohammadi, A. Kaviani, Water shortage and seawater desalination by electrodialysis, Desalination 158 (2003) 267-270
[20] T. Mohammadi, A. Moheb, M. Sadrzadeh, A. Razmi, Separation of copper ions by electrodialysis using Taguchi experimental design, Desalination 169 (2004) 21-31
[21] K.A. Al-Shayji, Modeling, simulation and optimization of large-scale commercial desalination plant, PhD thesis, Virginia Polytechnic Institute and State University, Virginia, USA, 1998
[22] J.A. Freeman and D.M. Skapura, Neural Networks Algorithms, Applications, and Programming Techniques, Addison-Wesley, Reading, Massachusetts, USA, 1992
[23] M. Sadrzadeh, A. Razmi, T. Mohammadi, Separation of different ions from wastewater at various operating conditions using electrodialysis, Separation and Purification Technology 54 (2007) 147-156

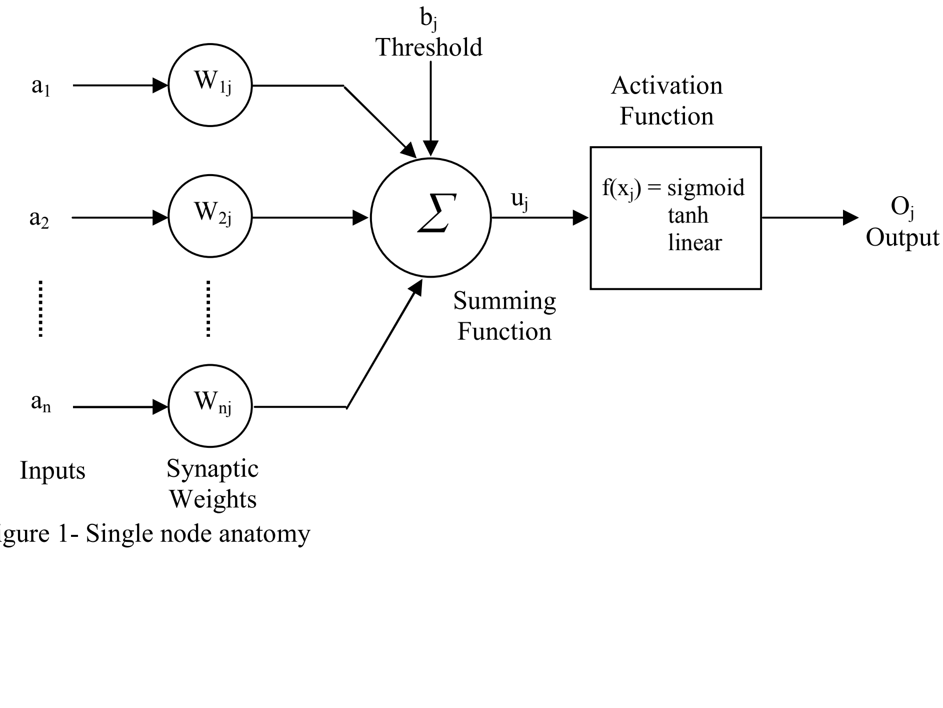


Figure 1- Single node anatomy

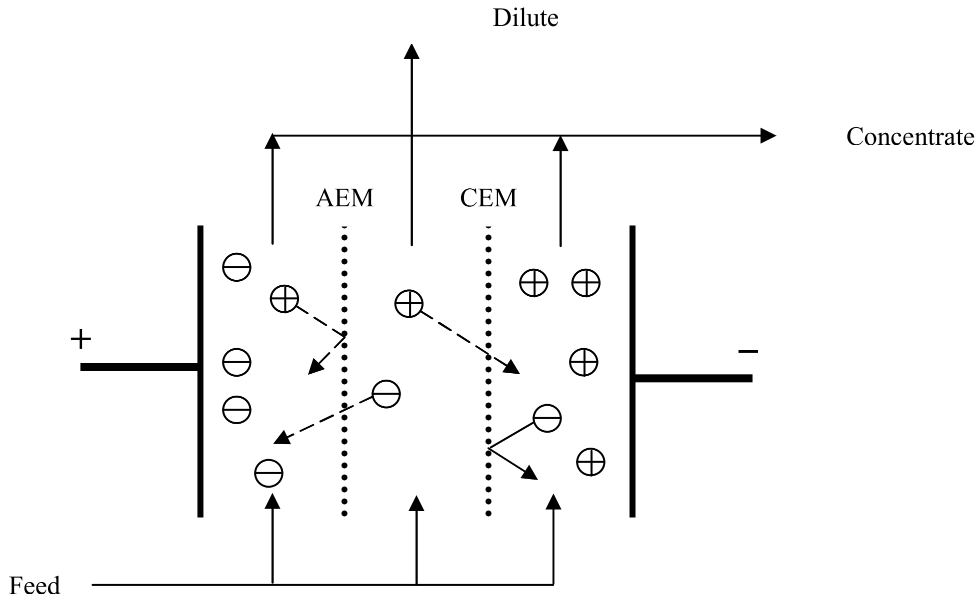


Figure 2- Schematic view of an ED cell

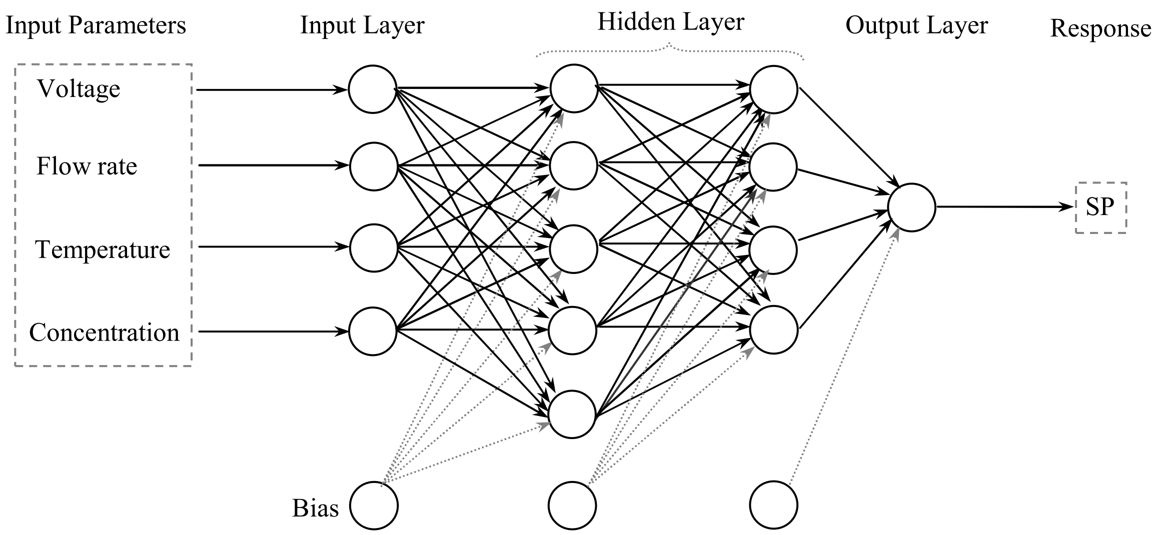


Figure 3- Structure of a typical ANN used for modeling of ED

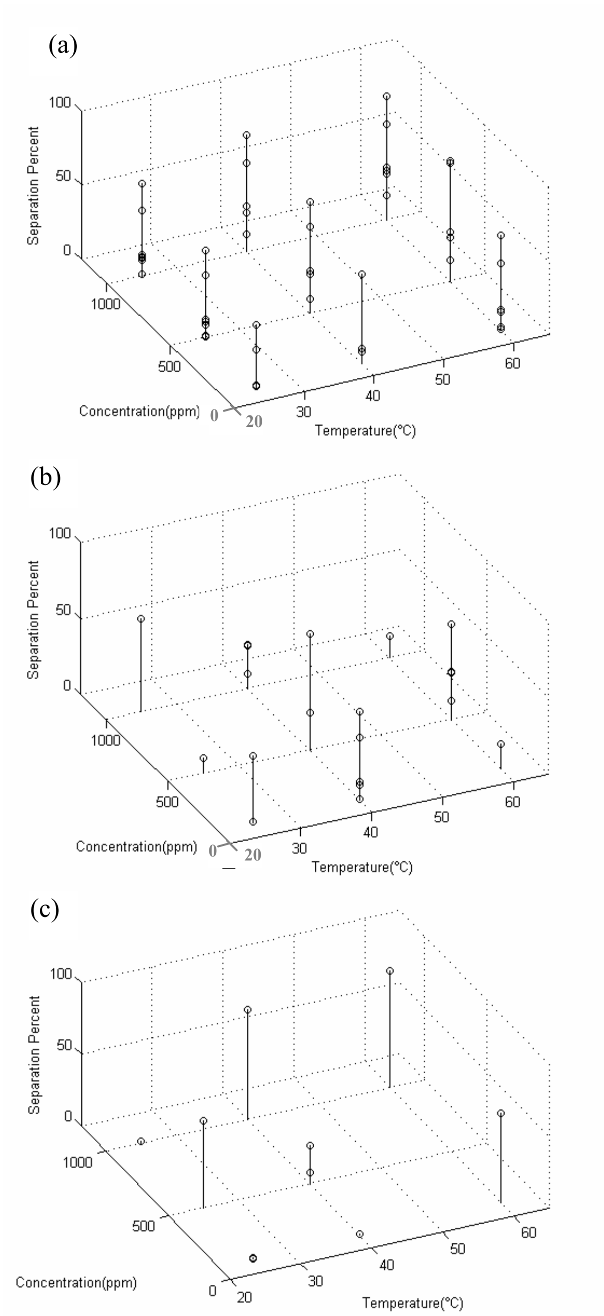
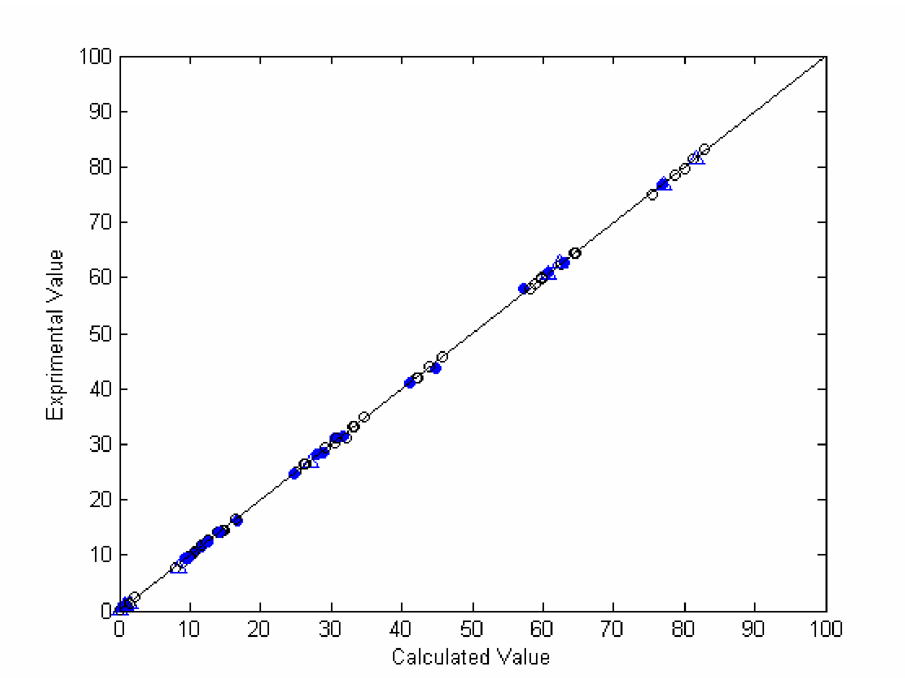


Figure 4- Distribution of (a) training, (b) validation and (c) testing data subsets



○: Training data ●: Validating data △: Testing data

Figure 5- Performance of 4:5:4:1 network at the minimum MSE of validation data

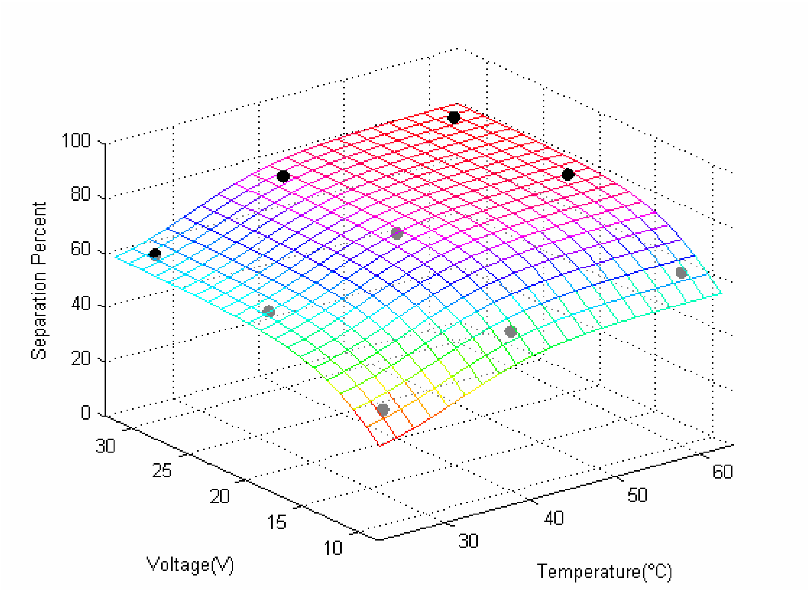


Figure 6- Generalization performances of optimal ANN, effects of voltage and temperature on SP at 500 ppm feed concentration and 0.07 mL/s feed flow rate

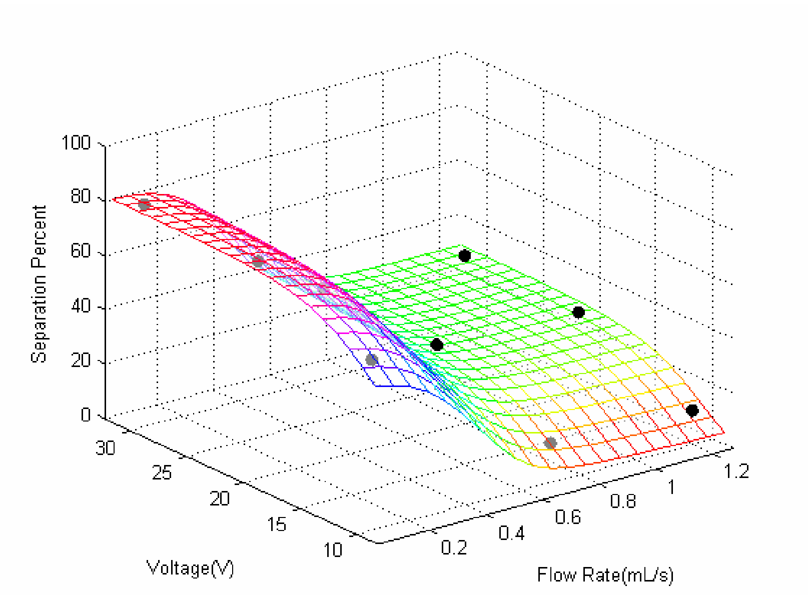


Figure 7- Generalization performances of optimal ANN, effects of voltage and flow rate on SP at 500 ppm feed concentration and 60 °C feed temperature

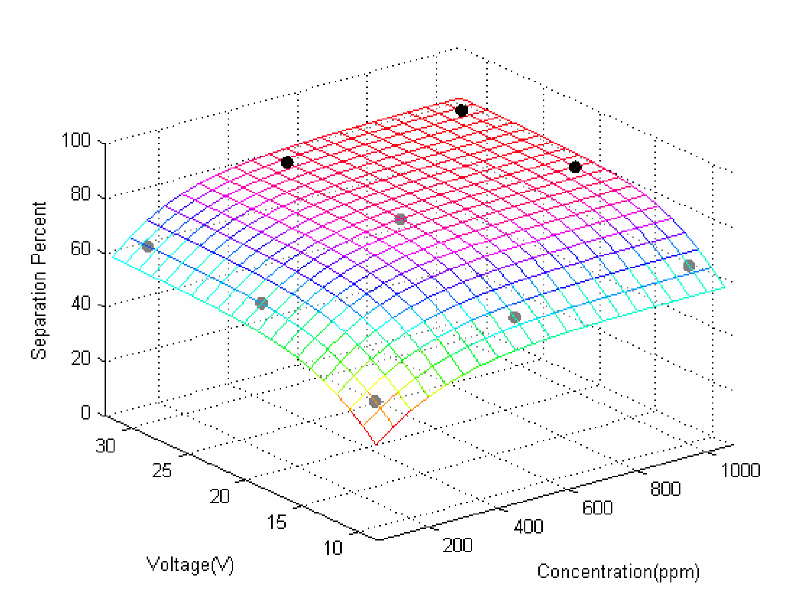


Figure 8- Generalization performances of optimal ANN, effects of voltage and Concentration on SP at 0.07 mL/s feed flow rate and 60 °C feed temperature