

An Artificial Neural Network Approach for the Prediction of Extraction Performance of Emulsion Liquid Membrane

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Abstract

This paper reports the use of artificial neural networks (ANN) approach to predict nickel concentration in external phase during emulsion liquid membrane extraction process. Experimental data from laboratory batch analysis of nickel extraction have been used to train, validate and test the back-propagation ANN model. The input neurons correspond to, external phase pH, stripping phase concentration, stirring speed, carrier concentration, surfactant concentration, treatment ratio (volume ratio of emulsion to external phase), phase ratio (volume ratio of membrane to stripping phase), initial external phase nickel(II) concentration, and time. A three-layer network with different hidden neurons and different learning algorithms such as LM, SCG, and BR were examined. The network with six hidden neurons and Bayesian regularization (BR) algorithm showed good performance. The predicted values of solute concentration in external phase are found to be in good agreement with the experimental results, with average absolute deviation (ADD%) of 0.2664% and correlation coefficient R^2 of 0.977. The results of this study show that the ANN model trained on experimental measurements can be successfully applied to the rapid prediction of external phase concentration

Keywords: Artificial neural networks; Emulsion liquid membrane; Prediction; External phase concentration

Introduction

Many methods have been used in waste water treatment generated by industrial processes such as solvent extraction, electro coagulation, activated carbon adsorption, ion exchange, emulsion liquid membrane (ELM), etc. Extraction processes using ELM, invented by Li [1] in 1968, have received significant attention for their potential as a technique for treatment of industrial liquid wastes due to its some attractive features for example, simultaneous performance of extraction and stripping in one stage, high efficiency, larger interfacial area [2]. Principally, emulsion liquid membrane involves a dispersion of emulsion water/oil (w/o) type containing organic and aqueous stripping phase into the aqueous feed (external) phase containing solutes to form double emulsion water-in-oil-in-water (w/o/w) type. A thin film of oil is formed between the outer (feed aqueous) phase and inner (stripping aqueous) phase, through which the complex solute-extractant, formed at the interface of the emulsion globule and the feed phase, diffuses and then is stripped into the encapsulated phase. The transportation of solute in the emulsion liquid membrane is chiefly motivated by the concentration gradient and pH [3].

A number of mathematical models have been developed over the years to describe the mechanism of solute transfer through emulsion liquid membranes. These models can be classified into the (1) the well-mixed internal phase or membrane film model (such as spherical shell model, plan film membrane) and (2) the rigid drop model or the distributed resistance model (such as advancing front and reversible model) [4]. The first model is based on the assumption that the entire resistance to mass transfer is assumed to be concentrated in a membrane film of constant thickness surrounding the emulsion globule. On the other hand, the second model is based on the assumption that the mass transfer resistance is to be distributed throughout the emulsion drop [5-10].

Emulsion liquid membrane process depends on several parameters such as external phase pH, stripping phase concentration, stirring speed, extractant concentration, surfactant concentration, treatment ratio (volume ratio of emulsion to external phase), phase ratio (volume ratio of membrane to stripping phase) and initial external phase concentration.

The development of mathematical models describing the process has proven to be difficult. The use of purely empirical models, which do not require any postulates and assumptions, appear to be new alternatives. One such method is the artificial neural network (ANN) approach. Extensive research has been performed with ANN approach in chemical engineering modeling [11-20]. In the present work an artificial neural network was developed to construct a predictive model to forecast the external phase concentration during emulsion liquid membrane extraction process. The details of the artificial neural networks are found elsewhere; however, a brief description is presented in Section 2.

Artificial Neural Networks

Artificial neural networks generally consist of a number of interconnected neurons or nodes that are organized in one or more layers. Rather than being programmed, neural networks can learn from exemplars, and have been shown to be effective in representing nonlinear relationships among variables [20]. Although different architectures have been reported, the uses of back propagation neural networks are particularly widespread in chemical engineering research, among others, owing to their simplicity, compact design and flexibility [11-18]. In back propagation neural networks (which have been used in this investigation), neurons are arranged in input, hidden, and output layers and linked to others with associated weights and biases, which will be adjusted to optimal values during the training. Collectively these connections, as well as the transfer functions of the processing units,

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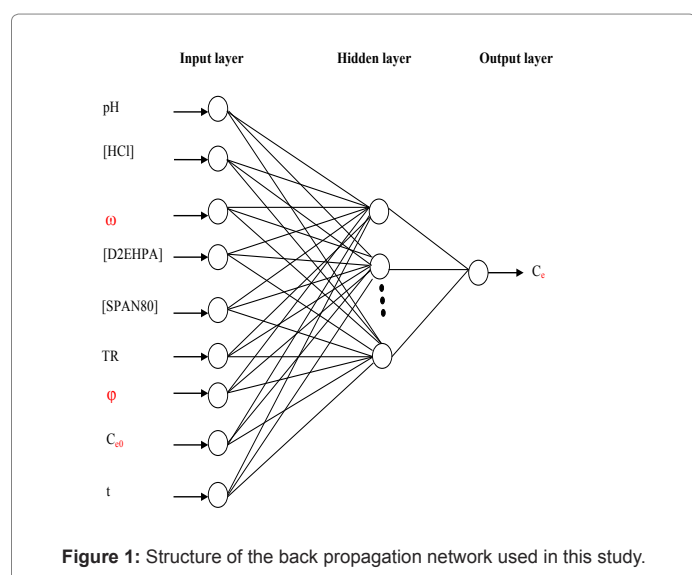
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can form distributed representations of relationships between input and output data.

Back propagation neural net training, is accomplished by repeatedly presenting the network with sets of exemplars of the process being modelled. During this supervised training process, the weights of the network are adjusted continuously based on the error signal generated by the discrepancy between the output of the network and the actual output of the training exemplars. The training process is accomplished by means of learning algorithms designed to minimize the mean square output error between the desired and actual output of the net [19,20]. The network is said to have converged when its outputs correspond closely with the desired outputs of the training data based on some arbitrary error criterion. The only task of the neurons in the input layer is to distribute the input signal to neurons in the hidden layer. The neurons in the hidden layer perform two tasks: they sum the weighted inputs connected to them and pass the resulting summations through a non-linear activation function (such as a sigmoid, or a hyperbolic tangent function) to the output neuron or adjacent neurons of the corresponding hidden. The output of neurons in the output layer is computed in the same manner. Following this calculation, a learning algorithm is used to adjust the strengths of the connections in order to allow a network to achieve a desired overall behaviour. There are many types of learning algorithms in the literature (Table 1). However, it is very difficult to know which training algorithm will be more efficient for a given problem [21].

Results and Discussion

The back propagation network employed in this modelling problem (Figure 1) consisted of an input layer with nine nodes corresponding to the operating variables: external phase pH, stripping phase concentration (hydrochloric acid: [HCl]), stirring speed (ω), carrier concentration (bis-(2-ethylhexyl) phosphoric acid: [D2EHPA]), surfactant concentration (Sorbitane monooleate: [Span 80]), treatment ratio TR (volume ratio of emulsion to external phase), phase ratio ϕ (volume ratio of membrane to stripping phase), initial external phase nickel(II) concentration (C_{e0}), and time (t), one hidden layer and an output layer with one node corresponding to the external phase Ni(II) concentration (C_e). The ranges of change in variables involved in extraction process are summarized in Table 2.



The experimental data used in this study to develop the ANN model are adopted from our published work [22], in which, effects of these operating variables (Table 2) on the extraction rate of nickel from chloride solution using ELM containing di-2-ethylhexyl phosphoric acid (D2EHPA) as a carrier in kerosene were examined. Thus database of the 245 data sets, was partitioned manually into three segments for training, validation and testing: 60% (185 data sets) were used to train the ANN models in order to determine network parameters, 10% (30 data sets) were used to cross-validate the relationships established during the training process (in order to monitor training progress so as to keep the network from overfitting) and the remaining 15% (30 data points) were used to test the ANN models to measure the performance of the predictive capability of the ANN after complete training. Before training, all input and target data were scaled to a similar magnitude in the range [-1,1] in order to convert them to a suitable form.

The Neural Network Toolbox available in MATLAB is implemented in this study to design and train the neural network. The back-propagation network was trained according to Bayesian regularization (BR) algorithm. Sigmoid and linear functions are assigned the transfer functions in hidden and output layers, respectively. The configuration of trained neural network is accomplished in terms of weights and bias values of each layer after the training and validation of construct networks [23].

To check the accuracy of the models in this study, statistical parameters such as mean relative error (MRE), mean square error (MSE) and average absolute deviation (AAD) are used. MRE, MSE and AAD are defined as follow:

$$MRE = \frac{1}{n} \sum_{i=1}^n \frac{(C_{e_{exp,i}} - C_{e_{pre,i}})}{C_{e_{exp,i}}} \quad (1)$$

$$MSE = \frac{1}{n} \sum_{i=1}^n (C_{e_{exp,i}} - C_{e_{pre,i}})^2 \quad (2)$$

$$AAD\% = \frac{1}{n} \sum_{i=1}^n 100 \times \left| \frac{C_{e_{exp,i}} - C_{e_{pre,i}}}{C_{e_{exp,i}}} \right| \quad (3)$$

Where, $C_{e_{exp}}$ and $C_{e_{pre}}$ are the experimental and predicted value, respectively. n is the number of samples.

Under the ANN modelling approach, the determination of optimal

Algorithm	Abbreviation	Description
Powell–Beale conjugate gradient algorithm	CGB	Generally, has a faster rate of convergence
Adaptive learning rate algorithm	GDX	Faster than basic gradient descent algorithm
Scaled conjugate gradient algorithm	SCG	The conjugate gradient algorithm requires no line search
BFGS quasi-Newton method	BFG	Usually converges in fewer iterations but requires estimating Hessian matrix
Levenberg–Marquardt algorithm	LM	One of the fastest training algorithms for networks of moderate size
Bayesian regularization	BR	Modification of the Levenberg–Marquardt algorithm to produce networks that generalize well

Table 1: The learning algorithms with brief descriptions used to train the ANN [22].

Measures parameters	Minimum	Maximum
Inputs		
External phase pH	2.98	4.02
Stripping phase concentration [HCl] (M)	0.5	2
Stirring speed ω (rpm)	200	700
Carrier concentration [D2EHPA] (%v/v)	2	10
Surfactant concentration [Span80] (%v/v)	2	10
Treatment ratio (TR)	0.1	0.2
Phase ratio (ϕ)	0.5	1.5
Initial nickel concentrationon C_{e0} (ppm)	100	594
Elapsed time (t) (s)	0	30
Outputs		
External phase concentration (C_e) (ppm)	0.875	249.6

Table 2: Range of experimental variables used for modelling.

Input weights	pH	[HCl]	ω	[D2EHPA]	[Span80]	TR	ϕ	C_{e0}	t	Bias
No. of neurons										
1	-0.1985	0.056	-0.1522	-0.0328	-0.0656	0.1827	-0.2461	-0.48	2.5371	0.8132
2	0.1382	-0.0703	-0.0737	0.098	0.0412	0.0288	-0.0874	-0.5777	1.9789	1.3611
3	0.7173	-0.2277	0.2875	0.4728	0.143	-0.6638	0.7802	-1.5882	-1.1008	-0.8033
4	-0.2265	0.0166	0.2367	-0.3027	0.1751	0.4046	-0.4454	3.1904	-0.0987	0.9857
5	-0.8044	0.3226	-0.2952	-0.5878	0.2854	0.6144	-0.6457	3.9371	-0.215	0.5915
6	-0.6096	0.3608	0.2575	-0.2966	0.2166	-0.4213	0.4988	-1.9773	-0.1966	-0.506
Neurons	1		2	3	4		5	6		Bias
Layer weights	0.9257	-1.6312		0.9474		-1.7554	1.5809		-2.1903	0.0478

Table 3: Optimum weights and biases for the used ANN model.

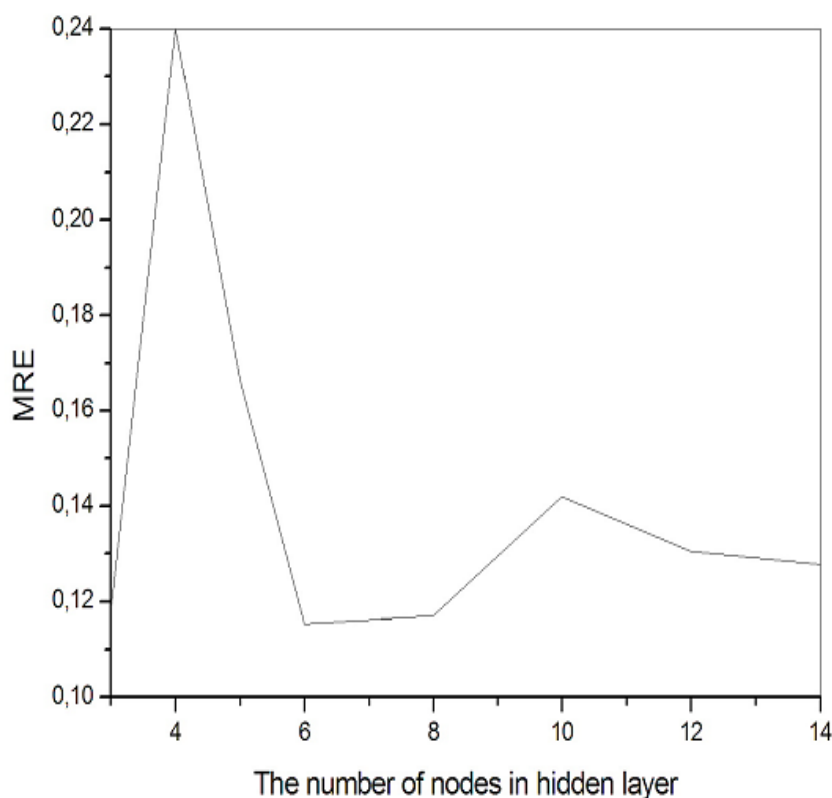


Figure 2: The hidden layer node numbers vs. MRE error on the validation set.

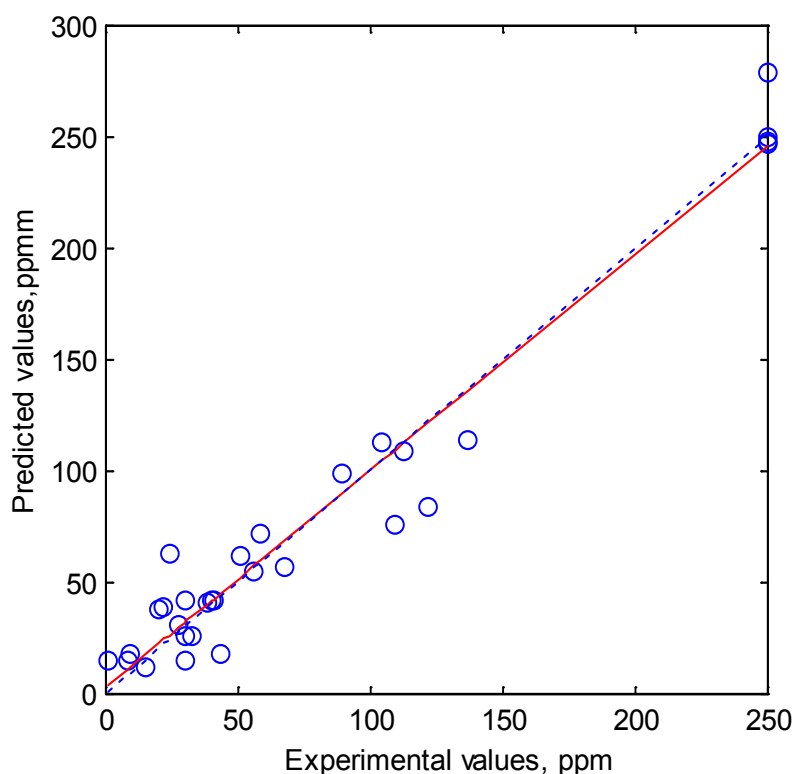


Figure 3: Evaluation of ANN performance; A scatter plot of typically measured experimental data against the ANN model for unseen data: ($R^2=0.978$, AAD%=0.2664).

Algorithm	MSE of network Training
Trainlm	2.3326e-006
Trainrb	1.2829e-005
trainscg	1.0617

Table 4: MSE Comparison between different algorithms for the training of ANN.

number of neurons in the hidden layer of the network is an important step. The number of neurons in the hidden layer has been optimized through minimizing the mean relative error (MRE) for the network trained with respect to the cross-validation data when the number of hidden neurons is varied (Figure 2). Based on this figure, it can be seen that six is the best number of hidden layer nodes with the least cross-validation MRE of 0.1153. Too many hidden neurons may cause the neural network to be over learned and on the other side, fewer hidden neurons will not provide sufficient freedom for the network to accurately learn the problem behaviour.

The configuration of trained neural network is accomplished in terms of optimum weights and bias values of each layer after the training and validation of construct networks. These optimum values have been presented in Table 3.

In order to train network, the training function which updates network weight and bias through various algorithms must be selected initially. To do so, performances of different training algorithms were studied. The mean square error (MSE) for various algorithm training, base on the six neurons in hidden layer, is listed in Table 4. As shown in Table 4 the Bayesian regularization (RB) algorithm provides the minimum error for training the network, so trainrb was selected as the proper training algorithm in this study.

After training, the ANN, the models become ready for testing and evaluation of its performance. Performance efficiency of the network was evaluated using the measured and ANN estimated value. A scatter plot of typically measured experimental data against the ANN model predictions was shown in Figure 3. As shown in Figure 3, the predicted external phase concentrations of the testing set were in acceptable good agreement with those of the experimental data. Almost all data lay on the diagonal line, which confirms the accuracy of the ANN model with average absolute deviation AAD% of 0.266 and correlation coefficient R^2 of 0.978.

Conclusions

In this paper, the ability of the neural network model for predicting external phase concentration was examined. Several learning algorithms such as LM, SCG, and BR with different hidden neurons were tested. The results show that a model with BR algorithm and 6 hidden neurons has the minimum mean relative error percent. The results of this study show that the ANN model trained on experimental measurements can be successfully applied to the rapid prediction of external phase concentration.

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