Selection of zero-cost reactive material for

permeable reactive barriers: Neural networks adoptability

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ABSTRACT

Batch experimental results play an important role in the selection of superior reactive materials for the design of permeable reactive barriers, which are being extensively used, for ground water treatment operations. Consequently, there is a need to develop methodologies enabling one to determine batch reactor performance, for designing more efficient reactive material under various conditions of influent. This chapter explores the feasibility of implementing an artificial neural network model for simulating the performance of batch tests using acidic ground water, which is a common problem in coastal plains of the world. Based on historical data, the chosen designed model inputs were reaction time, pH, and reactive specific surface area and the output variables were one or more of the following, aluminium, calcium, and iron concentrations. The proposed neural network model was trained using experimental tests data obtained through 20 different near zero-cost reactive materials. Training was followed by validation with independent sets of performance data obtained from the same batch tests. In addition, a set of split data sets were used for cross-validation of the ANN model. Non-linear multi regression models were also presented for the chosen ions of interest for comparison purpose. Consequently, simulation results obtained were carefully analyzed based on qualitative understanding of batch process and were found to provide key insights for the selection of the material as a promising reactant for the design of permeable reactive barriers under varying input conditions. Furthermore, the influence of each preferred input variable on the selected output was particularly evaluated and sequenced by sensitivity analysis, confirming that the selected inputs signals are the important determinants of output estimate. Owing to the existing nonlinear and uncertain chemical reaction characteristics of reactive materials, the ANN models showed high superiority in data simulation compared with non-linear multi regression models.

Keywords—Zero-cost reactive media; Batch tests; Permeable reactive barrier; ANN Modeling; acidic ground water modelling; Passive treatment technologies;

# INTRODUCTION

Acidic groundwater results from the interactions of sulphide minerals particularly pyrite with oxygen and water. In coastal plains worldwide, these waters have common problem due to the existence of 130 lakh hectares of acid sulphate soils [1]. During recharge of groundwater by rainfall, release of acid from the acid sulphate soils has mobilised large amounts of iron and aluminium in groundwater [1] [2], increases the attack on concrete, steel infrastructure, clog pores of the soil with iron flocculates, and kill fish. Owing to the impacts on environment, the research on acid sulphate water has increased [3][4][5][6].

Permeable reactive barrier (PRB) is now widely accepted technology for the remediation of polluted groundwater. The selection of the best suitable materials as reactive media is also one of the most important factors [7]. The material should cause no adverse chemical reactions or byproducts when reacting with constituents in the contaminant plume and cost-effective over acceptable endurance. When the reactive materials come into contact with the acidic groundwater, through physical, chemical, and/or biological processes, including precipitation, sorption, and oxidation/reduction, it gets remediated by neutralising the pH. Due to the complex, series, and parallel chemical reactions involved in the PRB system, the understanding and selection of the novel reactive media is one of the most important practical tasks.

Artificial neural networks have proven to be an attractive mathematical tool to represent complex relationships and belong to the class of data focused approaches, where the data are used to determine the structure of the model with the advantages of adaptive learning, self-organization, and real-time operation. ANN models can generalize the highly nonlinear data and provide the desired results for the cases where behavior of the system is not understood. Due to these attractive features, neural networks are increasingly being applied in modeling, where intricate physio-chemical processes prevail. Numerous researchers adopted ANNs in the field of geo-environmental engineering; virtual soil laboratory experiments [8], porosity and permeability prediction [9], geotechnical properties [10], settlement of shallow foundations [11], contaminant prediction [12][13], waste solidification [14], and swelling behaviour [15].

In contrast, the conventional statistical methods are model driven and the structure of the model has to be determined first before the unknown model parameters can be estimated. These statistical techniques suffer from the limitations such as inadequate knowledge about the distribution of the data. Regrettably, the use of statistical techniques to predict the effects of PRB reactive materials is limited due to the poor understanding of the different processes, and complex parallel and series chemical mechanisms involved. In the present work, neural networks have been proposed to understand the acidic ground water interaction with reactive materials by predicting the ion concentrations. A comparative study was also presented with non-linear regression models. The usage of ANN models for the prediction of ion concentrations would be a helpful tool, to select the novel reactive barrier material, which could be used to predict their behaviour without extensive practical experimentation.

# STRATEGY

## **Experimental Description**

This work involved the batch testing of 20 alkaline materials for use in the PRB, with an emphasis on near-zero cost waste materials, including blast furnace slag, recycled concrete, flyash, calcite-bearing zeolitic breccia, limestone, limestone, oyster shells, and dredged shell material. Representative acidic water was collected from the Southeastern coast of the Indian Peninsula to run the batch tests (Figure 1) at laboratory temperature (15-21 ºC) and atmospheric pressure. The collected water at the field site was acidic (pH as low as 3) with high levels of Al (up to 55 g/m3) and Fe (up to 20 g/m3) (Table 1). The purpose of the batch tests is to test the suitability of the materials to neutralise the acidity and remove Al and Fe from the groundwater. During the experiment, the samples were collected carefully to avoid flow disturbance and were analysed immediately for pH. Samples were also collected for analysis by inductively coupled plasma atomic emission spectroscopy after 0 day,1 day, 7 day, and 28 day. The samples were filtered under pressure through a 0.45 m membrane and refrigerated in high density polyethylene bottles until analysed for major ions such as calcium, aluminium, and iron. Prior to batch experiments, the reactive specific surface area of chosen materials was determined in the laboratory.



Figure 1: Schematic diagram of batch tank

Table 1:Statistical parameters of batch experiments used in training, testing, and validation

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Parameter | Mode of Operation | T | pH | RSSA | Al | Ca | Fe |
| (day) |  | (m2/g) | (g/m3) | (g/m3) | (g/m3) |
| Minimum | Training | 0 | 3.02 | 0.40 | 0 | 2 | 0.12 |
|  | Testing | 0 | 3.02 | 0.40 | 0.40 | 2 | 0.18 |
|  | Validation | 0 | 3.02 | 10.00 | 0.50 | 2 | 0.75 |
|  |  |  |  |  |  |  |  |
| Maximum | Training | 28 | 12.24 | 717 | 55.40 | 870.40 | 9.65 |
|  | Testing | 28 | 11.04 | 700 | 55.40 | 258.90 | 20.00 |
|  | Validation | 28 | 12.24 | 717 | 55.40 | 820.60 | 10.12 |
|  |  |  |  |  |  |  |  |
| Mean | Training | 9.09 | 7.19 | 306.19 | 17.47 | 145.63 | 2.57 |
|  | Testing | 8.98 | 7.10 | 337.68 | 12.74 | 78.48 | 3.36 |
|  | Validation | 8.11 | 6.54 | 334.89 | 18.69 | 182.20 | 4.32 |
|  |  |  |  |  |  |  |  |
| Median | Training | 4 | 6.59 | 120 | 2.40 | 39.30 | 0.89 |
|  | Testing | 7 | 8.21 | 600 | 1.30 | 29.80 | 1.41 |
|  | Validation | 1 | 5.90 | 120 | 7.90 | 38.20 | 3.35 |
|  |  |  |  |  |  |  |  |
| Mode | Training | 0 | 3.09 | 600 | 55.40 | 2.00 | 6.45 |
|  | Testing | 1 | 3.02 | 600 | 1.20 | 6.70 | 6.51 |
|  | Validation | 1 | 0 | 717 | 0 | 0 | 0 |
|  |  |  |  |  |  |  |  |
| Standard deviation | Training | 11.44 | 3.66 | 303.63 | 22.26 | 223.49 | 2.72 |
|  | Testing | 11.28 | 2.52 | 309.33 | 20.16 | 78.42 | 4.32 |
|  | Validation | 11.60 | 3.60 | 337.95 | 21.16 | 294.47 | 3.37 |
|  |  |  |  |  |  |  |  |
| Kurtosis | Training | -0.87 | -1.72 | -1.93 | -1.24 | 4.32 | -1.07 |
|  | Testing | -0.71 | -0.97 | -2.03 | 0.05 | -0.86 | 8.43 |
|  | Validation | 0.30 | -0.77 | -2.44 | -0.89 | 2.11 | -1.12 |
|  |  |  |  |  |  |  |  |
| Skewness | Training | 0.96 | 0.15 | 0.18 | 0.79 | 2.23 | 0.83 |
|  | Testing | 1.03 | -0.65 | -0.01 | 1.37 | 0.74 | 2.69 |
|  | Validation | 1.40 | 0.79 | 0.28 | 0.88 | 1.78 | 0.48 |
|  |  |  |  |  |  |  |  |
| Count | Training | 98 | 98 | 98 | 98 | 98 | 98 |
|  | Testing | 45 | 45 | 45 | 45 | 45 | 45 |
|  | Validation | 9 | 9 | 9 | 9 | 9 | 9 |
|  |  |  |  |  |  |  |  |

## **Reaction pathways and observed phenomena**

Oxidation reactions with acidic groundwater in general are complex and usually, several intermediates are formed, and the rate of their formation can vary widely [16]. Variation in the nature of precipitates occurs from material to material, and some materials may form many of these precipitates, while others form none. The precipitated products in Eqs. 1–4 are likely to form due to the interaction of iron and aluminium with water and carbonates and the saturation of calcium carbonate in the groundwater with rising pH [16].

 (1)

 (2)

 (3)

 (4)

## **Neural network approach to model leachate concentrations**

ANN is a parallel distributed processor similar to biological neurons that has a natural propensity for storing experimental knowledge and making it available for use. The selection of architecture depends on the tasks to be performed. The network consists of an input layer which receives inputs from the system, a hidden layer which receives inputs from input layer neurons, and the output layer which receives data from hidden layers and passes its output to an external domain. Figure 2 shows the general layout of the process used in this study. For developing a neural model, the test considered as a batch reactor under the influence of varying sets of inputs, will respond by producing different sets of outputs. Such a model presumes no prior knowledge about the structure of the relationship that exists between the input and output variable of the system. At any supplied feed conditions, the appropriate values of the leachate concentrations for the chosen reactive materials present in the system, works in fact as ANN model.

Input layer (Normalized inputs)

Hidden layer weights

Hidden layer Activation

Output layer weights

Output layer Activation

Hidden layer weights (updated)

Output layer weights (updated)

Figure 2: Training strategy of feed-forward ANN

To train a neural network successfully, a representative set of learning data has to be prepared based on the available batch reactor experimental results. This step has a decisive influence on the quality of the approximation of the output concentrations, and as such on the accuracy of process modelling as well as on the usability of the network for knowledge generalisation. Taking into account the properties of the reacting system, the input vector consists of three variables, reaction time (T), pH, and reactive specific surface area (RSSA), whereas the output could be any one of the variables, aluminium, calcium and iron concentrations. The pH is possibly the most promising physical parameter for monitoring the ion concentration in the leaching process, and this depends on the reaction time and specific surface area. The selected output of ion concentrations forms the main focus of the study.

Prior to neural modeling, it is common practice to divide the data sets into two subsets; a training set to construct the neural network model, and an independent validation set to estimate model performance in the deployed environment [17]. However, dividing the data into only two subsets may lead to model overfitting. To avoid this, cross-validation [18] [19][20] is used as the stopping criterion in this work and, subsequently, the database is randomly divided into three sets: training, testing, and validation. In total, 64% of the data are used for training and 30% are used for validation. The remaining 6% of data are used for cross validation. ANN inputs and outputs were normalized to lie in the range of [-1, 1] using the corresponding maximum value to preserve the interpretation of the weights and prevent numerical overflows. The selection of architectural parameters can influence network training and predictions. As the internal network parameters, a learning rate of 0.5 and the momentum of 0.2 were considered to train, test and cross validate the network. The Matlab® source code incorporating the salient features described above was used to implement this artificial neural network system on a personal computer.

**D. Non-liner multi regression model leachate concentrations**

Multi regression, which is a multivariate analysis model, is used for predicting the set of predictor variables. The concept of regression analysis lies in the idea of predicting the scores of one dependent variable ** from the scores of one or several independent variables *1*, * 2,*…, * m* in an optimal way. Standard multiple regression can only accurately estimate the relationship between dependent and independent variables if the relationships are linear in nature. If the relationship between independent variables and the dependent variable is not linear, the results of the regression analysis will underestimate the true relationship. A short code of Matlab® was adopted to develop the MRL models for aluminium, calcium and iron ions.

## **Neural network approach to leachate ion concentration network**

During training, the network weights converge to values such that each input vector produces the desired output. The method of back propagation propagates back the output errors to the network by appropriately modifying the weight matrices. The generalized delta rule was used to adjust weights and bias and is explained with output xj of each unit i to j as,

xj = Cj wij + bj  (5)

where, Cj is the output of unit j, wij is the weight of the connection from unit i to unit j, bj is the bias of unit j.

The result is then put through a simple sigmoid function *f*(C) to generate a level of activity for the neuron and is given by,

 (6)

During the learning procedure, a vector of the net parameters (weights) *w*has been modified to minimise differences between the outputs predicted with the net, *C*, and outputs used for learning, *d* (Eq.7).

 (7)

# RESULTS AND DISCUSSION

## **Selection of suitable hidden neurons**

In the absence of any rigorous rules, the optimal number of neurons in a hidden layer was determined via trial and error by systematically considering different combinations of neurons in the hidden layer. As the number of neurons in the hidden layer of the network increases, the problem becomes more complicated and can cause the network to memorize, and perform well during training, but fails to generalize. In general, fewer the hidden neurons, the better the network's performance. Hence, to resolve the dilemma, a study is made on the impact of the number of hidden neurons on the performance of the network.

Figure 3 shows the mean absolute error between the predicted and experimental concentrations of selected ions along with epochs by increasing the number of neurons in the hidden layer from 1 to 11. As the number of neurons adds to the network the epoch size increases with higher error values. Using four hidden neurons, the number of iterations is less with its prediction error is not far from that of the network coupled with a smaller number of connection weights. Thus in the present work 4 hidden neurons, single hidden layered feed forward back propagation network (i.e 3-4-1) is adopted, and the designed optimal network is shown in Figure 4 with its process description given in Table 2**.**



Figure 3: Impact of hidden layer neurons on the RMS error

Table 2: Input, hidden and output for each neural network layer

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Performed task | No. of neurons  K | Layer | Input to neuron | Output from neuron |
| Ion concentration  (Al/Ca/Fe) | 3 | Input | xj j = 1, 2…..k | Cj = xj, j =1,2,…k |
| 11 | Hidden | xj = ∑ki-1 Ci wij + bj ,  j = 1, 2,…..k | Cj = 1/{1+exp(-xj )}  J = 1,2,…k |
| 1 | Output | xj = ∑ki-1 Cj wij + bo | Cj0= xj0 |

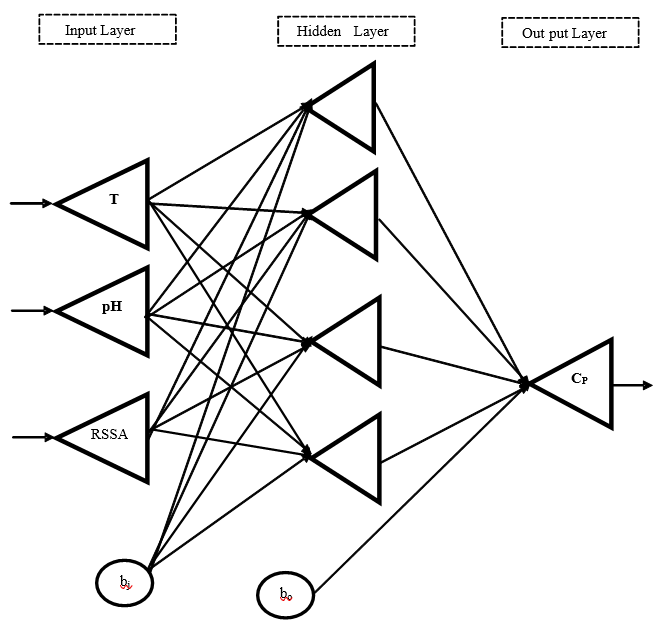


Figure 4: The designed ANN architecture for estimation of selected ion concentration

## **Prediction of ion concentration**

The performance measure values of the computed models for aluminium, calcium, and iron ions are shown in Table 3a and 3b. The stages of training include assembling the data, creating the network object; training the network, and simulating the network response to new inputs. The predicted and actual ion concentrations for training sets show a very strong correlation by r2 > 0.99 with RMSE errors as 1.0588, 19.9523, and 0.3258 for aluminium, calcium, and iron respectively. It can be noted from Figures 5-7 that almost all training data points lie on 1:1 line. The close correlation of the experimental and predicted leachate concentration of reactive materials with different pH and time periods indicates that the neural model is capable of memorizing the non-linear ion concentration to the multiple forcing signals of acidic water with reactive media.

 Figure 5: Correlation between experimental and predicted Aluminium concentrations



## Figure 6: Correlation between experimental and predicted Calcium concentrations



Figure 7: Correlation between experimental and predicted Iron concentrations

## Table 3a: Performance measures of neural network intelligence and regression models

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ion | Root mean square error | | | | | Mean sum square of the error | | | | |
| Artificial Neural Network | | | | Non-linear multiple regression | Artificial Neural Network | | | | Non-linear multiple regression |
| Training | Testing | Cross validation | Total | Total | Training | Testing | Cross validation | Total | Total |
| Al | 1.0588 | 1.5555 | 1.5227 | 1.2556 | 7.5944 | 1.1212 | 2.4195 | 2.3187 | 1.6917 | 57.6749 |
| Ca | 19.9523 | 22.5272 | 17.7374 | 20.6285 | 131.6876 | 398.0962 | 507.4734 | 314.6143 | 429.280 | 17341.6285 |
| Fe | 0.3258 | 0.4199 | 0.3303 | 0.3565 | 2.7008 | 0.1061 | 0.1763 | 0.1091 | 0.1311 | 7.2942 |

## Table 3b: Performance measures of neural network intelligence and regression models

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ion | Average relative error | | | | | r2estimate | | | | |
| Artificial Neural Network | | | | Non-linear multiple regression | Artificial Neural Network | | | | Non-linear multiple regression |
| Training | Testing | Cross validation | Total | Total | Training | Testing | Cross validation | Total | Total |
| Al | 0.6803 | 0.4777 | 0.4897 | 0.6165 | 4.9365 | 0.9977 | 0.9939 | 0.9942 | 0.9964 | 0.8753 |
| Ca | 2.0012 | 1.1663 | 0.0991 | 1.7278 | 2.6145 | 0.9919 | 0.9156 | 0.9959 | 0.9702 | 0.5590 |
| Fe | 0.3714 | 0.3218 | 0.0946 | 0.3466 | 1.5214 | 0.9855 | 0.9903 | 0.9892 | 0.9872 | 0.3359 |

## **Generalization of ion concentration**

The closeness of the points to the equality line (Figures 5-7) and the high values of r2 (0.9939, 0.9156, 0.9903) along with low values of MSSE (2.4195,507.4734,0.1763), RMSE(1.5555 g/m3,22.5272 g/m3, 0.4199 g/m3), and MAE (1.1306 g/m3, 20.01 g/m3, 0.2876 g/m3) clearly reflect the accuracy of the neural models for predicted concentrations ranging from 0.05 to 55.40 g/m3, 2 to 258.90 g/m3,and0.18 to 20 g/m3for aluminium, calcium, and iron concentrations, respectively. The performance outcome indicates that the back-propagation neural networks have the ability to generalize the ion concentrations of reactive materials, which are to be used as sorbing material in the PRB for treating acidic groundwater with an acceptable degree of accuracy.

## **Validation of ion concentration**

Prior to the usage of a developed model, there is a need to establish the validity of the results it generates. The chosen data sets have shown fairly good correlation (r2 = 0.9942; r2 = 0.9959; r2 = 0.9892) with the model predicted values for aluminium, calcium, and iron concentrations leading to the conclusion that the network could provide almost perfect answers to the set of problems with which it was trained (Figures 5-7).

To examine the overall performance, a comparative study was made between experimental, neural network, and regression models as shown in Figures 8-10. The r2 values are 0.88, 0.58, and 0.34 times less than those of the regression models, and the corresponding RMSE errors are 6.05, 6.40, and 7.58 times more for aluminium, calcium, and iron ions, respectively. This reveals that the ANN model performs reasonably well for the full range of measured ion concentrations of interest. In contrast, the regression methods only appear to work well in the range of 45-50 g/m3, 0-30 g/m3, and 0-1g/m3,for aluminium, calcium, and iron concentrations respectively.

## 

Figure 8: Variation of selected input parameters on output Aluminium concentration



Figure 9: Variation of selected input parameters on output Calcium concentration



Figure 10: Variation of selected input parameters on output Iron concentration

## **Effect of neutralization ability on ion concentration**

It can be observed from Figure 11, at nearly 3 pH the aluminium ion concentration is in the range of 42 to 58 g/m3, when acidic groundwater interacts with materials. As the experiment progressed, the neutralizing ability of the materials increased by releasing the calcium ions (Figure 12) and decreasing the aluminium ion concentration in the leachate. It could be due to the formation of aluminium hydroxide precipitates [16]. In addition, the formation of iron carbonates and iron hydroxide might have increased the pH of the materials in the leachate (Figure 13). The regression model was not able to perform for higher ion concentrations in the study.

## 

## Figure 11: Effect of pH on Aluminium concentration



## Figure 12: Effect of pH on Calcium concentration

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## Figure 13: Effect of pH on Iron concentration

## **ANN model equation for the selected ion concentrations (Cp) based on generalized neural network**

Neural networks have the advantage that once the model is trained, it can be used as an accurate and quick tool for estimating the concentration of ions without requiring further batch tests. In contrast, the shortcomings include the lack of theory to help with their development and the limited ability to explain the way they use the available information to arrive at a solution. The general mathematical form of equation as per the ANN relating the batch experimental inputs and the ion concentrations can be written as,

Concentration of ion, (8)

where Ck is the normalized (in the range of -1 to 1) Cp value; *f* is so-called the activation function; b0 is the bias at the out put layer; wki is the connection weight between Oth neuron of hidden layer and the single output neuron; bj is the bias at the hth neuron of hidden layer; h is the number of neurons in the hidden layer; wij is the connection weight between ith input variable and hth neuron of hidden layer; Xj is the normalized input variable j in the range [-1, 1]. The CP value as obtained from Eq. (8) is in the range [-1, 1] and this needs to be denormalized as,

CP = CP model (CP max – CP min) + CP min  (9)

where, CP = Predicted model selected ion concentration (g/m3); CP model = The model output; CP max = The maximum selected ion concentration (g/m3); and CP min = The minimum selected ion concentration (g/m3).

## **Proposed ANN model paramets Sensitivity analysis**

The sensitivity of neural network performance to the selected inputs was investigated to perceive how changes in an input variable affect the output variable. Figure 14 shows how sensitive the concentration of selected ions was at each of the selected input parameters, and how they would affect the changes. As expected, T, pH, and RSSAare the most important factors affecting the concentration of ions with an average relative importance equal to 32.21, 36.75, and 31.04%, respectively.



## Figure 14: Strength of input signal on output

I. **Non linear regression models for selected ion concentrations**

Regression allows one to form a multivariate regression relationship between a dependent variable and several independent variables. The multivariate regression model coefficients for dependent leachate ion concentrations are presented in Table 4 and the comprehensive multivariate regression model for dependent leachate concentrations is given by,

C = λi + i(βi(pH) + γi (RSSA) + 1i (T)2 + β1i (pH)2

+ γ1i (RSSA)2 + 2i (T)(pH)+ β2i (T)(RSSA)+ γ2i (pH)(RSSA) (10)

where, T is interaction time (day), pH is the hydrogen ion concentration, RSSA is the reactive specific surface area (m2/g).

# SUMMARY AND CONCLUSIONS

In this chapter, batch experimental results were used owing to the advantage of simplicity in experimentation and ease of operation in the selection of almost zero-cost superior reactive materials for the design of permeable reactive barriers, which are being extensively used as passive treatment, for ground water treatment operations. Neural network based aluminium, calcium, and iron simulation models were proposed and tested for applicability with the aid of batch reactor data, to predict the ion concentration in acidic groundwaters. The influence of each preferred input variable on the selected output was evaluated and sequenced by sensitivity analysis, confirming that the selected input signals are the significant determinants of the output estimate.

Table 4: Multivariate regression model coefficients for dependent leachate ion concentrations

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Model Ion Concentration | Model coefficients | | | | | | | | | |
| C | Λ |  | β | γ |  | β | γ1 |  | β | γ2 |
| Al | 107.948 | -1.3996 | -22.9693 | 0.0034 | 0.0203 | 1.1931 | -2.42e-05 | 0.0738 | 0.0002 | 0.0019 |
| Ca | 229.997 | 10.0136 | -103.1703 | 0.3872 | -0.2867 | 9.7983 | -0.0005 | -0.1934 | 0.0017 | -0.0147 |
| Fe | 8.992 | -0.3718 | -0.9268 | -0.0056 | 0.0040 | 0.0242 | 3.84e-06 | 0.0220 | 2.91e-05 | 0.0004 |

C = Ion concentration (g/m3)

 (10a)

 (10b)

 (10c)

Based on the study the following primary conclusions can be drawn.

1. The artificial neural network model (3-4-1) thus developed is able to generalize the ion concentrations of interest using interaction time, pH, and reactive specific surface area. All the statistical results confirm that neural networks are precise tools in the quantitative study of reactive materials in the complex acid groundwater system. Hence the ANNs can be used as a preliminary assessment tool for acid sulphate soil remediation.
2. Increase in the number of hidden layer neurons increases the network performance up to a definite level, and thereafter, the generalization capability reduces considerably.
3. The ion concentrations of interest obtained from chosen reactive materials by ANN technique shows a good correlation with batch tests (r2 = 0.9964, r2 = 0.9702, and r2 = 0.9872), leading to the conclusion that ANN is better applicable for complex problems than regression methods (r2 = 0.8753, r2 =0.5590, and r2 =0.3359) for aluminium, calcium and iron ions, respectively.
4. ANNs use the data alone to determine the structure and parameters of the model. In this case, there is no need to simplify the problem or incorporate any assumptions. Moreover, ANNs can always be updated to obtain better results by presenting new training examples as new data become available.

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