SELECTION OF ZERO-COST REACTIVE MATERIAL FOR PERMEABLE REACTIVE BARRIERS: NEURAL NETWORKS ADOPTABILITY

Abstract

The selection of superior reactive materials for the construction of permeable reactive barriers—which are widely utilized for ground water treatment operations—is heavily influenced by the findings of batch experiments. As a result, it is necessary to make procedures that make it possible to assess the performance of a batch reactor. As a consequence, methods for evaluating the performance of batch reactors must be devised in order to design reactive materials that are more effective under diverse influent conditions. This chapter investigates whether an artificial neural network model could be used to simulate the results of batch testing utilizing acidic ground water, a phenomenon that is prevalent in coastal plains all over the world. Reaction time, pH, and reactive specific surface area were selected as the intended model inputs based on historical data and the output variables were one or more of the following, aluminium, calcium, and iron concentrations. Utilizing experimental test data gathered from 20 different nearly cost-free reactive materials, the suggested neural network model was constructed. Following training, validation was conducted using various sets of performance data that were collected from the same batch of tests. The ANN model was also cross-validated using a collection of split data sets. For the selected ions of interest, non-linear multi regression models were also offered for comparison. In order to select a material as a potential reactant for the design of permeable reactive barriers under a variety of input conditions, simulation results were carefully examined based on a qualitative understanding of

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batch processes. Additionally, using sensitivity analysis, the impact of each preferred input variable on the chosen output was carefully assessed and ordered, demonstrating that the chosen input signals are the key factors influencing the estimate of the output. Due to the reactive materials' existing nonlinear and ambiguous chemical reaction properties, ANN models outperformed non-linear multi regression models in terms of data simulation.

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

I. INTRODUCTION

Acidic groundwater is a global issue caused by the interactions of sulphide minerals such as pyrite with oxygen and water. This problem is especially pervasive in coastal plains, where over 130 million hectares of acid sulfate soils exist[1]. During the recharge of groundwater from rainfall, the release of acid from acid sulfate soils has caused significant mobilization of iron and aluminum 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].

In order to clean up contaminated groundwater, a device termedas permeable reactive barrier (PRB) is now often employed. The selection of suitable materials to utilize as reactive mediums is one of the most crucial factors [7]. The material shouldn't cause any adverse chemical reactions or byproducts when interacting with elements of the polluted plume, and it should be affordably priced for a sufficient period of time. By bringing the reactive materials into touch with the acidic groundwater through precipitation, sorption, oxidation/reduction, and other physical, chemical, and/or biological processes, it is remedied by bringing the pH level back down. 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.

Adaptive learning, self-organization, and real-time operation make artificial neural networks an appealing mathematical tool for representing complex relationships. They fall under the category of data focused approaches, where the data are used to determine the model's structure. When the system's behavior is unclear, ANN models may generalize the highly nonlinear data and deliver the required outcomes. Because of these appealing qualities, neural networks are being used more and more in modeling, where complex physio-chemical processes are common. 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 structure of the model must be established before the unknown model parameters may be estimated using the traditional statistical approaches. These statistical methods are constrained by things like a lack of understanding of the manner in which the data are distributed. Unfortunately, due to the complexity of the parallel and series chemical reactions involved and the lack of a thorough knowledge of multiple processes, the application of statistical tools to forecast the effects of PRB reactive materials is confined. 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 useful approach to choosing the unique reactive barrier material that could be used to forecast their behavior without requiring substantial practical investigation is the use of ANN models for the prediction of ion concentrations.

II. STRATEGY

1. **Experimental Description:** This investigation comprised batch testing for use in the PRB of 20 alkaline materials, with a focus on near-zero cost waste materials, such as blast furnace slag, recycled concrete, flyash, zeolitic breccia carrying calcite, limestone, oyster shells, and material from dredging shells.Throughout the batch experiments (Figure 1), representative acidic water was collected from the Indian Peninsula's southeast coast. The testing was performed at atmospheric pressure and laboratory temperature (15–21^{o}C). The collected water at the field site was high in Al (up to 55 g/m^{3}) and Fe (up to 20 g/m^{3}) and acidic (pH as low as 3; Table 1). The primary objective of batch testing is to figure out whether the materials are suitable for neutralizing acidity and removing Al and Fe from groundwater. The samples were carefully collected during the experiment in order to avoid flow disruption, and the pH was determined right away. After 0 days, 1 days, 7 days, and 28 days, samples were also collected for analysis using inductively coupled plasma atomic emission spectroscopy. Prior to being analyzed for significant ions like calcium, aluminum, and iron, the samples were filtered under pressure through a 0.45 m membrane and preserved in high density polyethylene bottles in the refrigerator. The reactive specific surface area of the selected materials was calculated in the lab prior to batch trials.

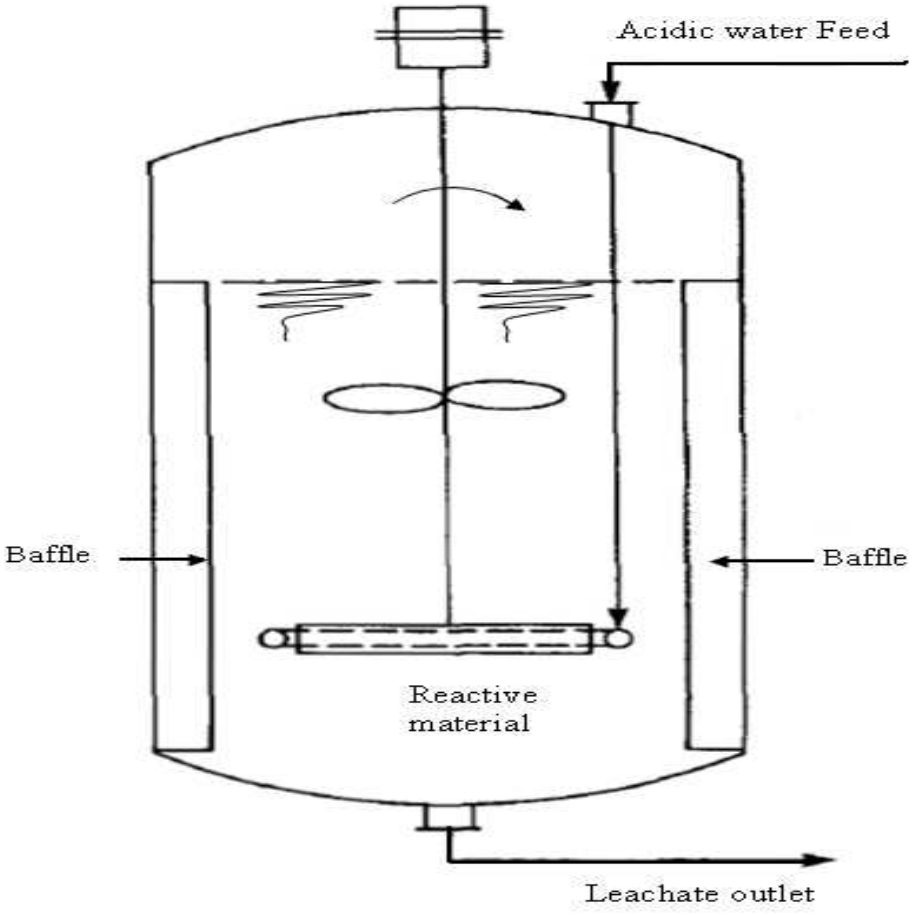

Figure 1: Schematic diagram of batch tank

Table 1: For training, testing, and validation, batch experiments' statistical parameters

Parameter	Mode of Operation	T	pH	RSSA	Al	Ca	Fe
		(day)		(m^2/g)	(g/m^3)	(g/m^3)	(g/m^3)
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

2. **Routes of Reactions and Observable Phenomena:** In general, oxidation processes with acidic groundwater are complicated, and often a number of intermediates are generated, often at varying rates [16]. Different materials form various kinds of precipitates, and while some materials may form many of these precipitates, others may not. The precipitated products in equations 1-4 are anticipated to occur as a result of calcium carbonate being saturated in the groundwater as a result of increased pH and the interaction of iron and aluminum with water and carbonates [16].

$$Fe^{2+} + 2OH^{-} \leftrightarrow Fe(OH)_{2(s)} \quad (1)$$

$$Fe^{2+} + CO_3^{2-} \leftrightarrow FeCO_{3(s)} \quad (2)$$

$$Al^{3+} + 3H_2O \rightarrow Al(OH)_{3(s)} + 3H^{+}_{(aq)} \quad (3)$$

$$Ca^{2+} + CO_3^{2-} \leftrightarrow CaCO_{3(s)} \quad (4)$$

3. **Neural Network Approach to Model Leachate Concentrations :** The parallel distributed processor called an ANN, which resembles biological neurons, has a built-in predisposition to store and make use of experimental knowledge. The selection of architecture depends on the tasks to be performed. The network is made up of an input layer that takes inputs from the system, a hidden layer that takes inputs from neurons in the input layer, and an output layer that takes data from hidden layers and sends its output to an outside domain. The general design of the procedure employed in this investigation is shown in Figure 2. For the purpose of creating a neural model, the test is considered as a batch reactor that responds to different sets of inputs by producing various sets of outputs. Such a model makes no assumptions about prior knowledge of the relationship's structure between the system's input and output variables. The suitable values of the leachate concentrations for the selected reactive components present in the system, at any provided feed circumstances, really function as an ANN model.

   A representative collection of learning data must be created based on the available batch reactor experimental findings in order to successfully train a neural network. This stage has a significant impact on the accuracy of process modeling, the applicability of the network for knowledge generalization, and the quality of the approximation of the output concentrations.The input vector contains three variables-reaction time (T), pH, and reactive specific surface area (RSSA)-while the output might be any of the three variables-concentrations of aluminum, calcium, or iron-depending on the characteristics of the reacting system. Depending on the reaction duration and particular surface area, the pH is maybe the most promising physical measure for monitoring the ion concentration in the leaching process. The chosen output of ion concentrations serves as the study's primary point of interest.

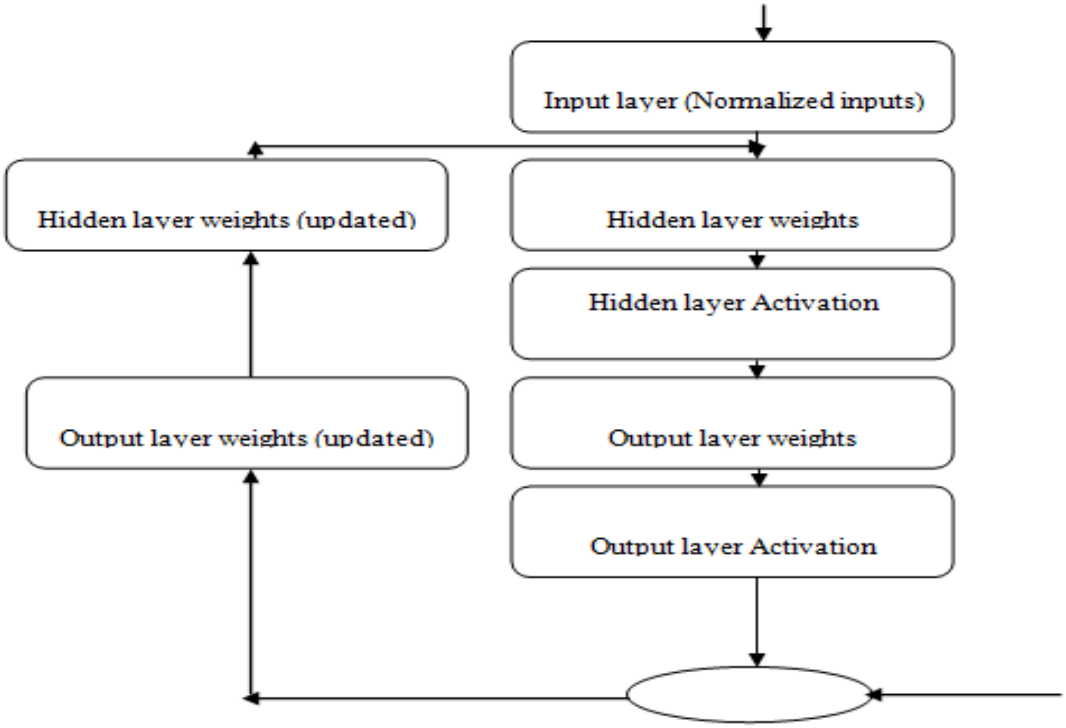

Figure 2: Training strategy of feed-forward ANN

It is a standard procedure to separate the data sets into two subsets before performing neural modeling: a training set for building the neural network model and an independent validation set for determining how well the model performs in the deployed environment [17]. Only splitting the data into two subsets, however, might result in model overfitting. To circumvent this, the database is randomly partitioned into three sets: training, testing, and validation. Cross-validation [18] [19] [20] is then employed as the stopping criterion in the present investigation. 30% of the data are used for validation, while the remaining 64% are used for training. The remaining 6% of data are used for cross validation. To maintain the meaning of the weights and avoid numerical overflows, ANN inputs and outputs were normalized to fall within the range of [-1, 1] using the associated maximum value. 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.

4. **Non-Liner Multi Regression Model Leachate Concentrations :** A multivariate analytic approach called multi-regression is utilized to forecast an assortment 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 ε_1, ε_2,…, $\varepsilon_m$in an optimal way.

Only linear relationships between dependent and independent variables can be used in standard multiple regression to assess the relationship between the variables. Regression analysis results tend to overstate the underlying relationship if there is a nonlinear relationship between the independent and dependent variables. A short code of Matlab® was adopted to develop the MRL models for aluminium, calcium and iron ions.

5. **Neural Network Approach to Leachate Ion Concentration Network:** The network weights converge to values during training such that each input vector yields the desired output. Through the appropriate modification of the weight matrices, the backpropagation approach feeds the output faults back into the network. The output x_j of each unit from i to j is used to demonstrate how the generalized delta rule was utilized to change weights and bias.

$$x_j = C_j w_{ij} + b_j \tag{5}$$

where, C_j is the output of unit j, w_{ij} is the connectionsweight from unit i to unit j, b_j is the bias of unit j.

The output is then passed through a straightforward sigmoid function, f(C), to provide an estimate of the neuron's degree of activity, which is given by,

$$f(C_j) = \frac{1}{1+e^{-C_j}} \tag{6}$$

A vector of the net parameters (weights) w has been altered during the learning process to minimize disparities between the outputs utilized for learning, d, and the outputs anticipated with the net, C (Eq. 7).

$$E(W) = \frac{1}{2}\sum_{j=1}^{P}\sum_{k=1}^{M}(C_k^{(j)} - d_k^{(j)})^2 \tag{7}$$

III. RESULTS AND DISCUSSION

1. **Selection of Suitable Hidden Neurons:** The appropriate number of neurons in a hidden layer was established by trial and error by methodically analyzing various combinations of neurons in the hidden layer in the absence of any strict criteria. The network may memorize information and perform well during training as the number of neurons in the hidden layer of the network rises, but the network may not be able to generalize as the problem becomes more complex. The performance of the network improves generally as the number of hidden neurons decreases. So, in order to find a solution to the problem, a study is done to determine how many buried neurons affect the network's performance.

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**.**

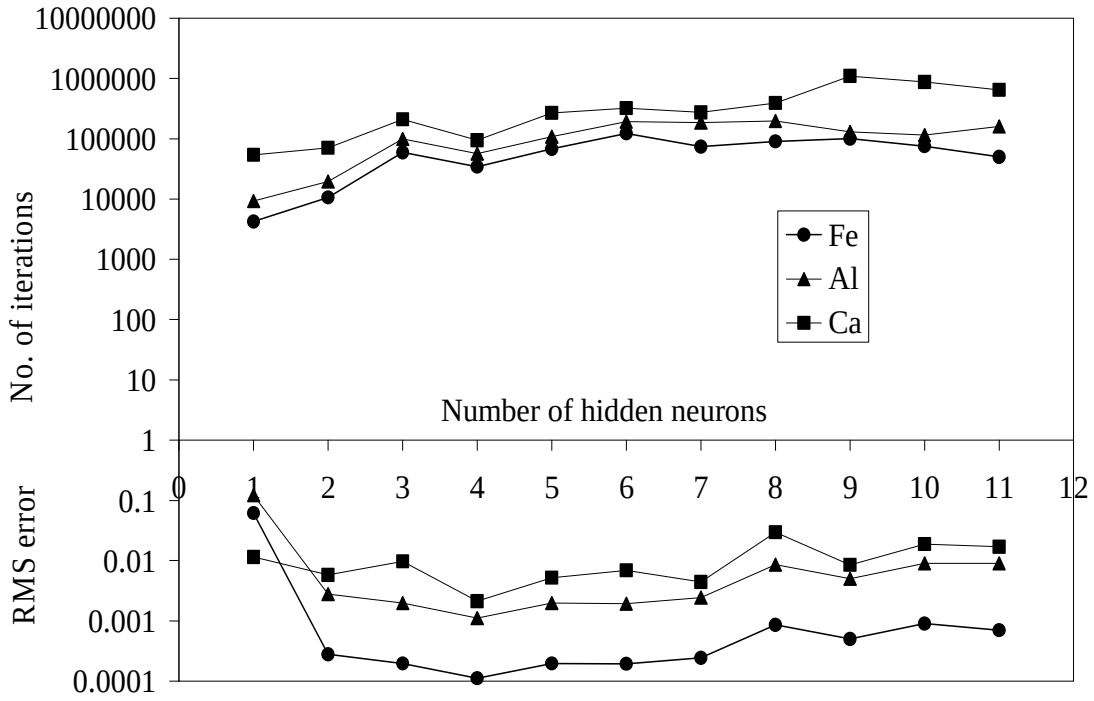

Figure 3: Impact of hidden layer neurons on the RMS error

Table 2: Each layer's input, hidden input, and output in a neural network

Performed task	Neuronsp resent K	Layer	Neuron's input	Output from neuron
Ion concentration (Al/Ca/Fe)	3	Input	x_j j = 1, 2…..k	$C_j = x_{j,}$ j =1,2,…k
	11	Hidden	$x_j = \sum_{i-1}^{k} C_i w_{ij} + b_j$, j = 1, 2,…..k	$C_j = 1/\{1+\exp(-x_j)\}$ J = 1,2,…k
	1	Output	$x_j = \sum_{i-1}^{k} C_j w_{ij} + b_o$	$C_j^0 = x_j^0$

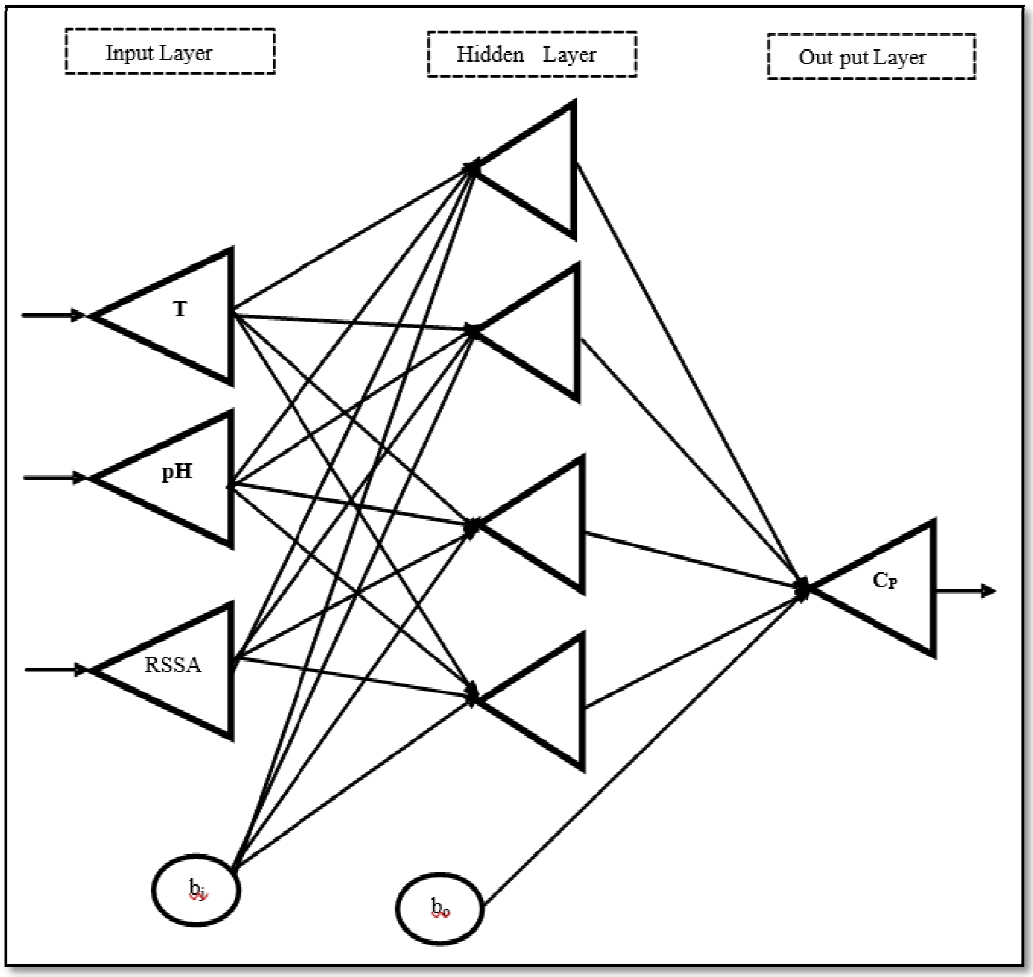

Figure 4: The designed ANN architecture for estimation of selected ion concentration

2. **Prediction of Ion Concentration:** The performance measure values of the computed models for aluminium, calcium, and iron ions are shown in Tables 3a and 3b. Assembling the data, developing the network object, training the network, and simulating the network's reaction to novel inputs are all phases of the training operation.The predicted and actual ion concentrations for the training sets exhibit a very strong correlation (r^2> 0.99), with the RMSE errors for the metals aluminum, calcium, and iron comprising 1.0588, 19.9523, and 0.3258, respectively. Figures 5-7 show that practically all training data points fall on the 1:1 line. The neural model is able to memorize the non-linear ion concentration to the numerous driving signals of acidic water with reactive media, as evidenced by the strong correlation between the experimental and predicted leachate concentration of reactive materials with varying pH and time periods.

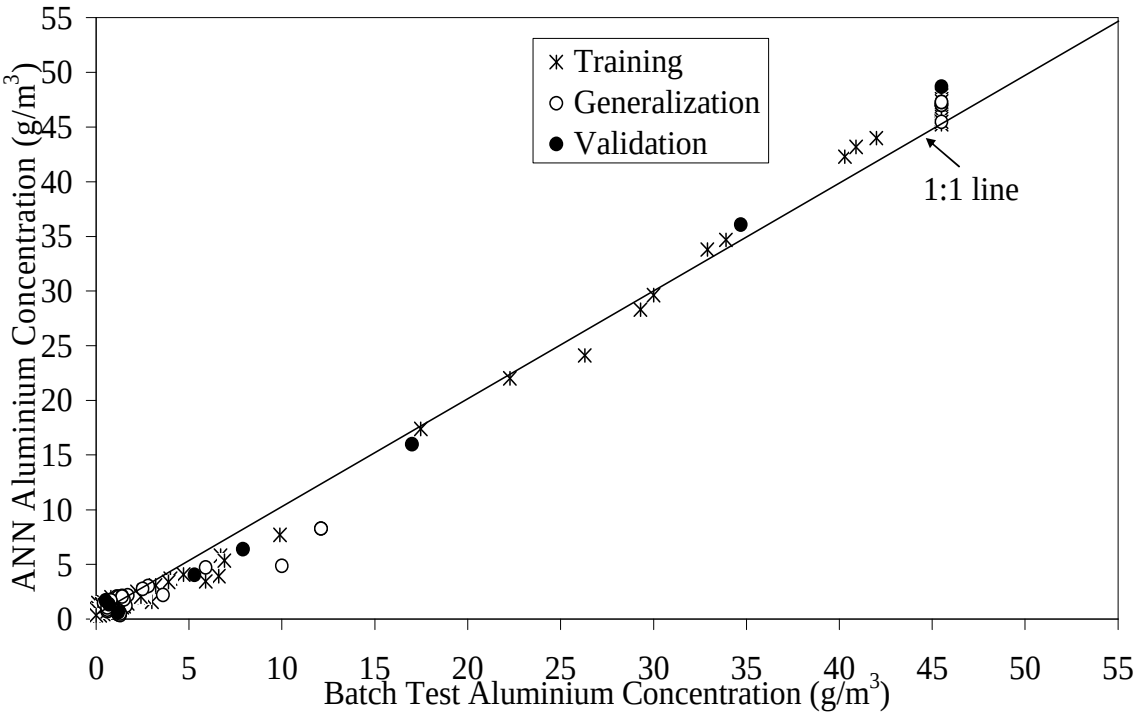

Figure 5: Correlation between experimental and predicted Aluminium concentrations

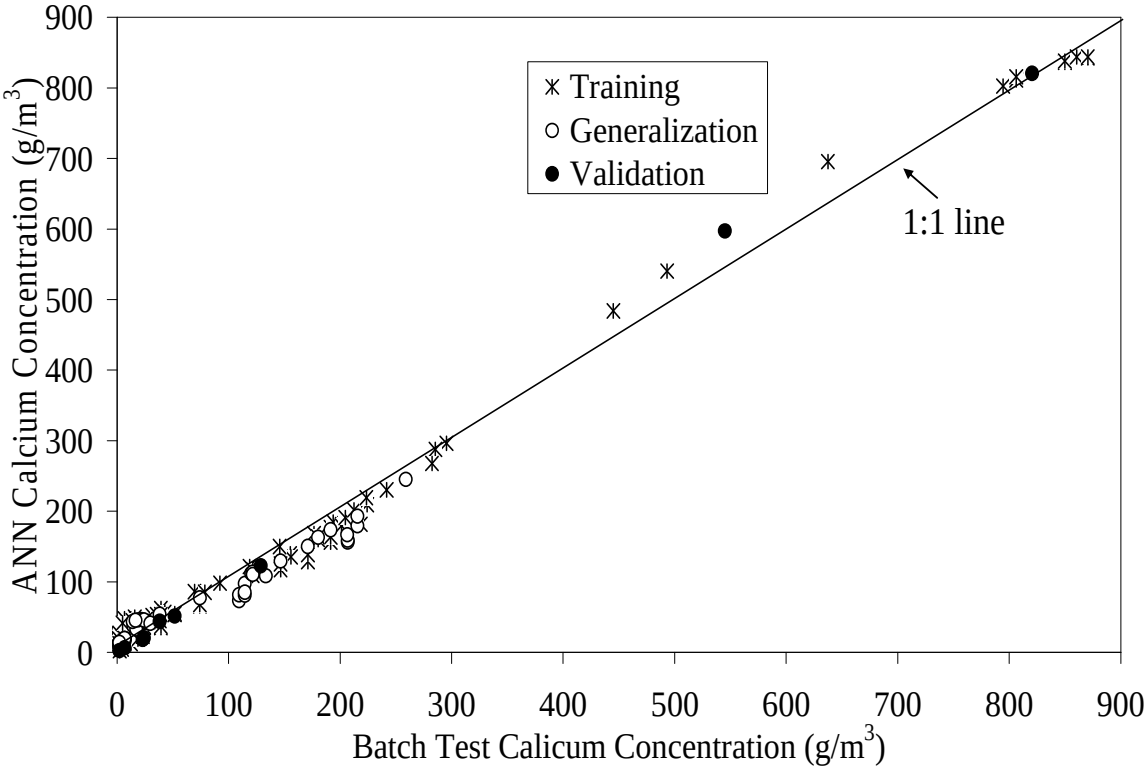

Figure 6: Correlation between experimental and predicted Calcium concentrations

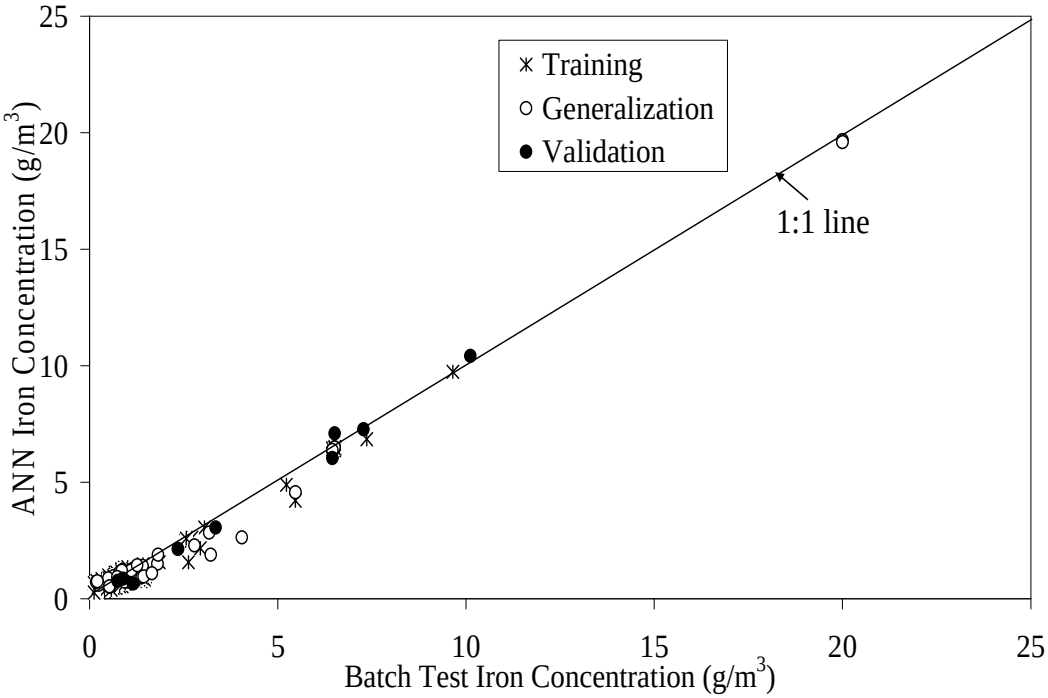

Figure 7: Correlation between experimental and predicted Iron concentrations

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					r^2 estimate				
	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

3. **Generalization of Ion Concentration:** The closeness of the points to the equality line (Figures 5-7) and the high values of r^2 (0.9939, 0.9156, 0.9903) along with low values of MSSE (2.4195,507.4734,0.1763), RMSE(1.5555 g/m^3,22.5272 g/m^3, 0.4199 g/m^3), and MAE (1.1306 g/m^3, 20.01 g/m^3, 0.2876 g/m^3) and the displayed concentrations of aluminium, calcium, and iron, which range from 0.05 to 55.40 g/m3, 2 to 258.90 g/m3, and 0.18 to 20 g/m3, respectively, clearly illustrate the accuracy of the neural models.Pursuant to the performance results, back-propagation neural networks are capable of predicting ion concentrations of reactive materials, which are to be employed as sorbing material in the permeable reactive barrier for treating acidic groundwater, with an adequate degree of accuracy.

4. **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 demonstrated fairly good correlation (r^2 = 0.9942; r^2 = 0.9959; r^2 = 0.9892). The network was able to provide nearly ideal solutions to the collection of problems with which it was trained, as shown by the anticipated values for the concentrations of iron, calcium, and aluminum (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 r^2 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 rather well over the whole range of relevant observed ion concentrations. For aluminum, calcium, and iron concentrations, respectively, the regression approaches only seem to function well in the

range of 45-50 g/m^3, 0-30 g/m^3, and 0-1 g/m^3.

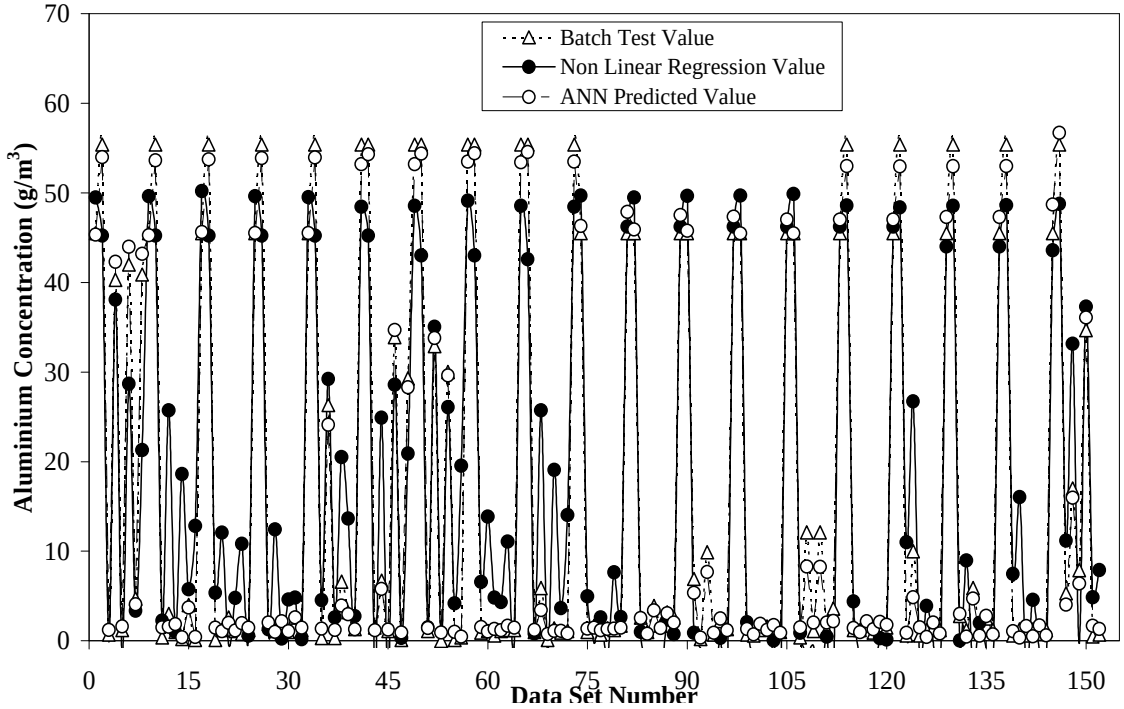

Figure 8: Variation of selected input parameters on output Aluminium concentration

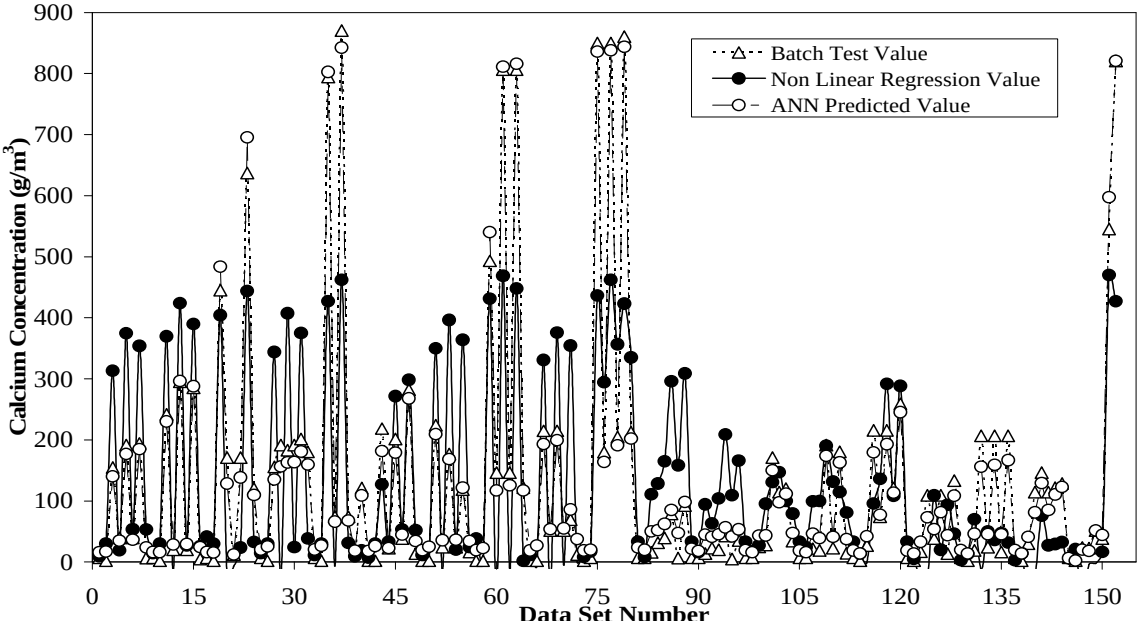

Figure 9: Variation of selected input parameters on output Calcium concentration

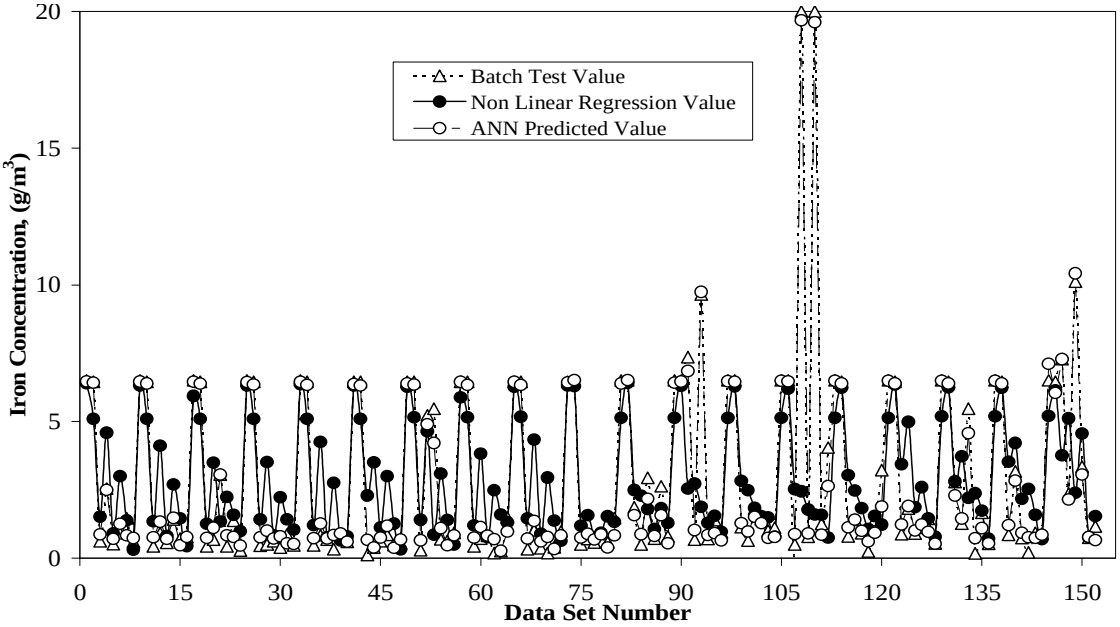

Figure 10: Variation of selected input parameters on output Iron concentration

5. **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/m^3, 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.

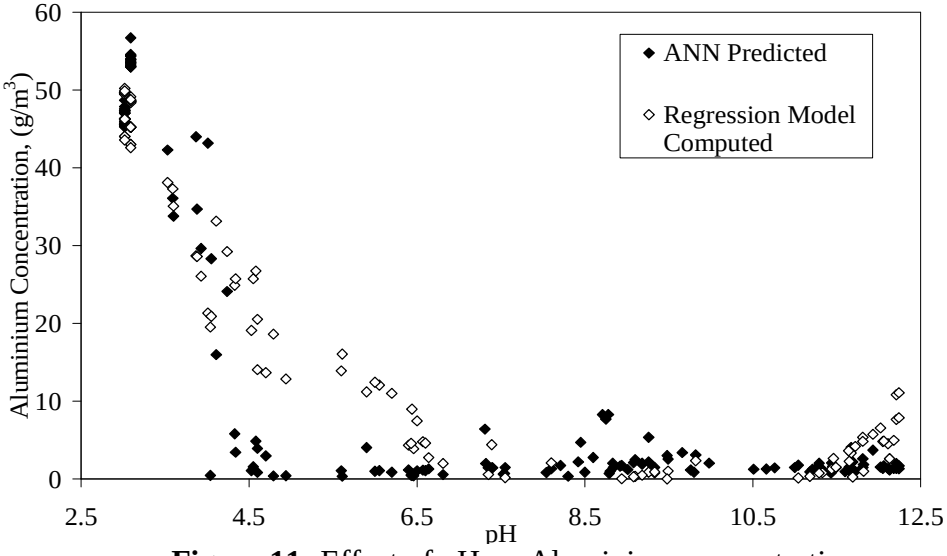

Figure 11: Effect of pH on Aluminium concentration

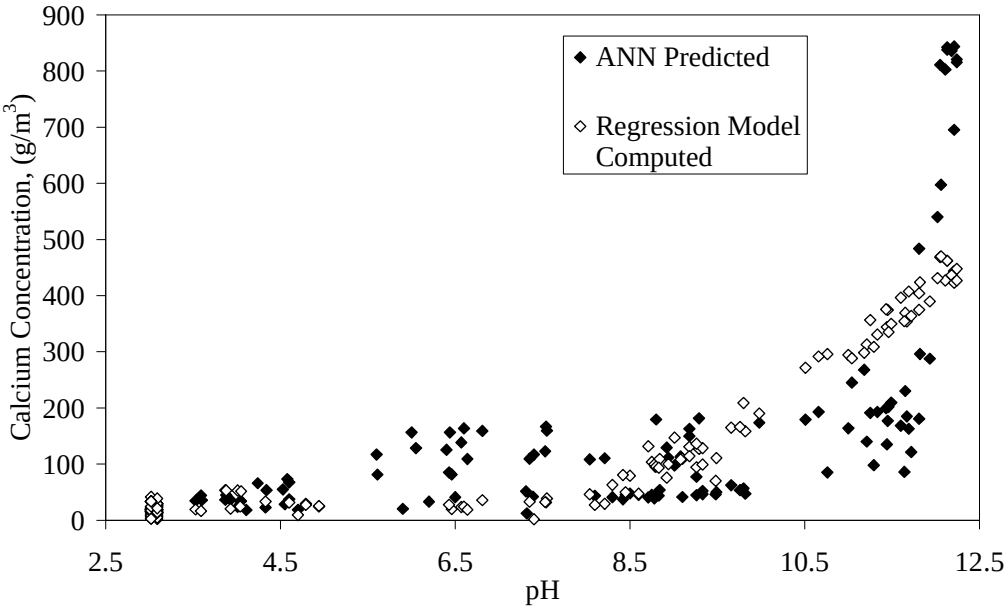

Figure 12: Effect of pH on Calcium concentration

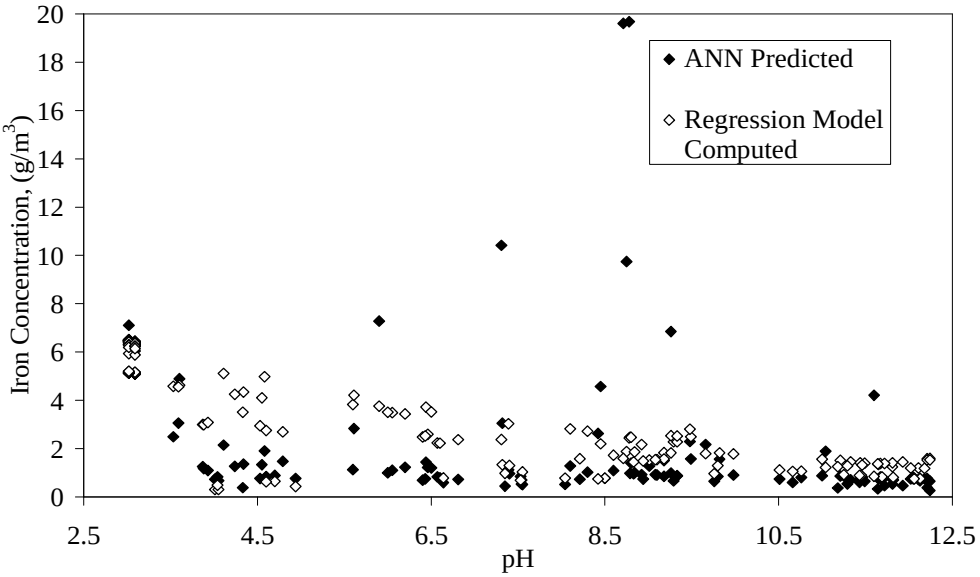

Figure 13: Effect of pH on Iron concentration

6. **ANN Model Equation for the Selected Ion Concentrations (C_p) Based on generalized Neural Network:** The benefit of neural networks is that, after training, they can be utilized as a quick and accurate tool to estimate the concentration of ions without the need for additional batch tests. The drawbacks, on the other hand, include a lack of theory to aid in their development and a limited capacity to describe how they employ the facts at hand to come up with 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,

$$\text{Concentration of ion, } C_k = f\left[\sum_{i=0}^{K} W_{ki}^{(O)} f\left(\sum_{j=0}^{N} W_{ij}^{(h)}.X_j + b_j\right) + b_o\right] \quad (8)$$

where h is the number of neurons in the hidden layer, C_k is the normalized C_p value (in the range of -1 to 1), f is the so-called activation function, b_0 is the bias at the output layer, w_{ki} is the connection weight between the eighth hidden layer neuron and the single output neuron, b_j is the bias at the h^{th} hidden layer neuron, w_{ij} is the connection weight between the i^{th} input variable and the h^{th} hidden layer neuron, The range of the C_P value as determined by Eq. (8) is [-1, 1], and thus needs to be denormalized as,

$$C_P = C_{P\,model}\,(C_{P\,max} - C_{P\,min}) + C_{P\,min} \tag{9}$$

where, C_P = Predicted model selected ion concentration (g/m^3); $C_{P\,model}$ = The model output; $C_{P\,max}$ = The maximum selected ion concentration (g/m^3); and $C_{P\,min}$ = The minimum selected ion concentration (g/m^3).

7. **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.

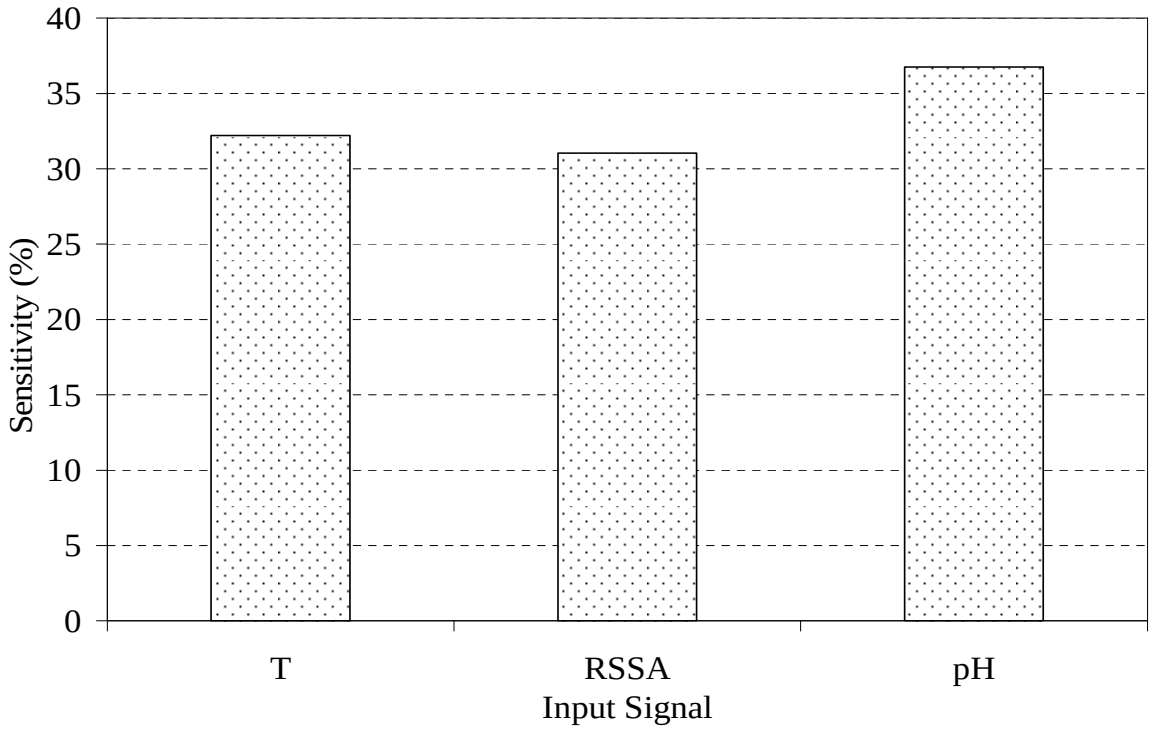

Figure 14: Strength of input signal on output

8. **Non Linear Regression Models for Selected Ion Concentrations:** A dependent variable and numerous independent variables can be related in a multivariate way using regression. 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,

$$C = \lambda_i + \alpha_i (T) + \beta_i (pH) + \gamma_i (RSSA) + \alpha 1_i (T)^2 + \beta 1_i (pH)^2 + \gamma 1_i (RSSA)^2 + \alpha 2_i (T)(pH) + \beta 2_i (T)(RSSA) + \gamma 2_i (pH)(RSSA) \quad (10)$$

where, T is interaction time (day), pH is the hydrogen ion concentration, RSSA is the reactive specific surface area (m^2/g).

IV. SUMMARY ANDCONCLUSIONS

Owing to the advantages of simplicity in experimentation and ease of use in the selection of almost cost-free superior reactive materials for the design of permeable reactive barriers, which are widely used as passive treatment, for ground water treatment operations, batch experimental results were used in this chapter. With the help of batch reactor data, neural network-based simulation models for predicting the ion concentration in acidic groundwaters were created and tested for applicability. Sensitivity analysis was used to evaluate and rank the effects of each desired input variable on the chosen output, indicating that the chosen input signals are the important factors influencing the output estimate.

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

Model Ion Concentration	Model coefficients									
C	Λ	α	β	γ	α1	β1	γ1	α2	β2	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/m^3)

$$C_{Al}(g/m^3) = 107.9481 - 1.3996(T) - 22.9693(pH) + 0.0034(RSSA) + 0.0203(T)^2 + 1.1931(pH)^2 - 0.00001(RSSA)^2 + 0.0738(T)(pH) + 0.0002(T)(RSSA) + 0.0019(pH)(RSSA) \quad (10a)$$

$$C_{Ca}(g/m^3) = 229.9974 + 10.0136(T) - 103.1703(pH) + 0.3872(RSSA) - 0.2867(T)^2 + 9.7983(pH)^2 - 0.0005(RSSA)^2 - 0.1934(T)(pH) + 0.0017(T)(RSSA) - 0.0147(pH)(RSSA) \quad (10b)$$

$$C_{Fe}(g/m^3) = 8.992 - 0.37181(T) - 0.92682(pH) - 0.0056355(RSSA) + 0.0040127(T)^2 + 0.0242(pH)^2 + 3.841e-006(RSSA)^2 + 0.021968(T)(pH) + 2.9138e-005(T)(RSSA) + 0.00039647(pH)(RSSA) \quad (10c)$$

Based On the Study the Following Primary Conclusions Can be Drawn.

- The artificial neural network model (3-4-1) created in this way uses interaction time frame, pH, and reactive specific surface area to generalize the desired ion concentrations. 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.
- An increase in hidden layer neurons improves network performance up to a certain degree, but after that, generalization ability of ionic concentrations drastically decreases.
- The ion concentrations of interest obtained from chosen reactive materials by ANN technique shows a good correlation with batch tests (r^2 = 0.9964, r^2 = 0.9702, and r^2 = 0.9872), leading to the conclusion that ANN is better applicable for complex problems than regression methods (r^2 = 0.8753, r^2 =0.5590, and r^2 =0.3359) for aluminium, calcium and iron ions, respectively.
- The structure and parameters of the model are decided by ANNs purely based on the data. There is no need to formulate any assumptions or simplify the problem in this instance. As new data comes available, ANNs can also be upgraded to produce even better results by showing additional training examples.

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