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EVALUATING PORTLAND CEMENT CONCRETE DEGRADATION BY SULPHATE EXPOSURE THROUGH ARTIFICIAL NEURAL NETWORKS MODELING

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ABSTRACT

A concrete is durable if it has accomplished the desired service life in the environment in which it is exposed. The durability of concrete materials can be limited as a result of adverse performance of its cement-paste matrix or aggregate constituents under either chemical or physical attack. Among other aggressive chemical exposures, the sulphate attack is an important concern. Water, soils and gases, which contain sulphate, represent a potential threat to the durability of concrete structures. Sulphate attack in concrete leads to the conversion of the hydration products of cement to ettringite, gypsum, and other phases, and also it leads to the destabilization of the primary strength generating calcium silicate hydrate (C-S-H) gel. The formation of ettringite and gypsum is common in cementitious systems exposed to most types of sulphate solutions. The present work presents the application of the neural networks for estimating deterioration of various concrete mixtures due to exposure to sulphate solutions. A neural networks model was constructed, trained and tested using the available database. In general, artificial neural networks could be successfully used in function approximation problems in order to approach the data generation function. Once data generation function is known, artificial neural network structure is tested using data not presented to the network during training. This paper is intent to provide the technical requirements related to the production of a durable concrete to be used in the structures of the Brazilian near-surface repository of radioactive wastes.

1. INTRODUCTION

Concrete could be used to build huge structures as bridges, tunnels, dams, sewerage systems, and more. Its cost and high performance for most purposes are two of many factors that contribute to concrete to be the most used man-made material in the world. Concrete structures are required to have high durability and serviceability. The problem faced by the engineers who prepare specifications for concrete for particular work is to predict the deteriorative influences that could cause degradation of concrete in service in the environment at the project site over the intended service life of the concrete [1]. A concrete is durable if it has accomplished the desired service life in the environment in which it is exposed. The durability of concrete materials can be limited as a result of adverse performance of its cement-paste matrix or aggregate constituents under either chemical or physical attack.

Sulphate ions present in soil, groundwater, and sea water can cause deterioration of reinforced Portland cement concrete structures due to sulfate attack. But what is sulphate attack? The use of the term '*sulphate attack*' has promoted most of the research efforts to focus on the effects of the SO_4 ion alone. As a matter of fact, attack by different sulphate solutions, such as the ones containing Ca, Na, Mg, and Fe as the cation, proceeds differently with respect to the mechanism and the type of distress caused [2]. Upon the penetration of sulphate ions into the concrete, the calcium monosulfoaluminate crystals in the paste may convert into gypsum or ettringite. It results in a change to a larger molar volume, and these volumetric changes cause expansion and internal stresses, which ultimately weaken and destroy the paste bonds, deteriorating the concrete, particularly affecting surface layers, which increases the exposure conditions for interior concrete. Both sodium and magnesium sulphates contribute to sulphate attack, with their effectiveness regulated by the presence of other ions in solution. Solutions containing magnesium sulphate have been shown to be more detrimental than solutions containing the same concentration of sodium sulphate because both $SO_4^{\ 2-}$ and Mg^2+ contribute to the damage [3]. Despite the research in this area, a prediction model does not exist. Therefore, Artificial Intelligence (AI) computational analysis techniques arise as a possibility of solution.

Artificial Neural Networks (ANN) are algorithms simulating biological nervous system, and may be used to solve problems that conventional computations modeling techniques find difficult to solve. Neural networks are networks of many simple processes, which are called units, nodes, or neurons, with dense parallel interconnections. The connections between the neurons are called synapses. Each neuron receives weighted inputs from other neurons and communicates its outputs to other neurons by using an activation function. Neural networks might be single-or multilayered. The single-layer neural networks present processing units of the neural networks, which take input from the outside of the networks and transmit their output to the outside of the networks; otherwise, the neural networks are considered multilayered [4]. Generally, the neural network is created for two phases, referred to as the '*Training phase*' and the '*Reproduction phase*'. During the training phase sample data containing both inputs and desired outputs are processed to optimize the network's output in order to minimize deviation. The neural network is operated using back-propagation networks, which generally have a layered structure with an input layer, an output layer, and one or more hidden layers (layers that may contain a large number of hidden processing units). Units in the input layer represent the possible influential factors that affect the network outputs and have no computation activities, while the output layer contains one or more processing units that produce the network outputs. Propagation takes place in a feed-forward manner from the input layer to the output layer, compares the network outputs with known targets, and propagates the error back to the network using a learning mechanism to adjust the weights and biases. In order to construct neural network model the first thing to do is to establish the network architecture. Once it is accomplished, the degree of success of the neural network model in prediction largely depends upon how comprehensive the training data is [5]. This study is intent to show the effect of sulphate exposure on the performance of Portland cement concretes. In this regard, experimental techniques (compressive strength, ultrasonic pulse velocity, and mercury intrusion porosimetry tests), and an ANN modeling will be presented. It is part of ongoing research to provide the technical requirements related to the production of a durable concrete to be used in the structures of the Brazilian near-surface repository of radioactive wastes.

2. METHODS AND MATERIALS

2.1. Materials

Two concrete mixtures were prepared for the study: C20 (with characteristic compressive strength f_{ck} at 28 days of 20 MPa) and C50 (with characteristic compressive strength f_{ck} at 28 days of 50 MPa). The test specimens were cast according to the NBR-5738 Brazilian Standard Test Method [6]. The materials used for the fabrication of the two concrete mixtures were:

- tap water;
- river sand with finesses modulus of 2.27 as fine aggregate;
- 19 mm maximum sized calcitic limestone (CC), dolomitic limestone (CD), and gneiss (GN) as coarse aggregate;
- Brazilian Portland cement CP II-E-32 (equivalent to ASTM Type I (SM)(MS)), CP III-32-RS (equivalent to ASTM Type IS (MS)), and CP IV-32 (equivalent to ASTM Type IP (MS)) as binder;
- lignosulphonate based plasticizer admixture of 945 ml/m^3 for C20 mixture and 1940 ml/m^3 for C50 mixture as water reducer;
- silica fume of 55,5 kg/m^3 for C50 mixture as solid addictive;

The amount of concrete specimens to be molded depended on certain variants as the type of cement, type of coarse aggregate, magnesium sulphate compositions, and time of immersion of concrete on sulphate compositions. Thus, three groups of four specimens were molded, giving a total of twelve specimens for each mixture; the total number of molded specimens was 648. Twenty-four hours after casting the specimens were demouded and part of them immersed in tanks with three different magnesium sulphate ($MgSO_4$) compositions of 0 g/l (just water), 10 g/l, and 50 g/l solutions. In order to simulate wet and dry cycle the specimens were kept in the solution for 1 day and let to dry for 3 days; the wet-dry cycle was repeated continuously for 28 days, 90 days, and 180 days. A more detailed description is available in Costa [7].

2.2. Tests

2.2.1. Ultrasonic pulse velocity

Ultrasonic pulse velocity tests were performed in order to determine the concrete inner porosity. The time of travel of an ultrasonic pulse wave from a transmitter to a receiver was the chosen parameter to achieve it. The tests were carried out using portable ultrasonic non-destructive digital-indicating testers PUNDIT 6 and V-Meter Mark II, with flat transducers in accordance with NBR-8802 Brazilian Standard Test Method [8].

2.2.2. Mercury intrusion porosimetry

Mercury intrusion porosimetry tests were performed in order to determine the concrete surface porosity. The medium pore diameter was the chosen parameter to achieve it. The tests were conducted using an AutoPore III 9220 V 3.05 (Micromeritics) porosimeter, capable to produce pressures up to 420 MPa. Small pieces of sample were collected on the surface of concrete specimens and had their aggregates removed. The samples were dried before testing in an oven at 130°C for 24 hours.

2.2.3. Compressive Strength

The uniaxial compressive strength tests were performed in accordance with the procedure proposed in the NBR-5739 Brazilian Standard Test Method [9]. The concrete specimens were capped by sulfur mortar.

3. NEURAL NETWORKS MODELING

A Sigmoid function was chosen after considering the entire available experimental results database. Sigmoid function is a mathematical function having an "S" shaped curve, and frequently refers to the special case of the logistic function. It is depicted in **Figure 1**. The Sigmoid function used is ranged between 0 and 1, and it is defined by the Equation (1):

$$f(u) = \frac{1}{1+e^{-\beta u}} \tag{1}$$

Since the experimental results are out of the reference range, normalizing the output was required prior to presenting them to the network. Normalization means adjusting values measured on different scales to a notionally common scale, and it is necessary whenever there is the need to harmonize the outputs. In the present study the database should have the *minimum* and *maximum values* of 0 and 1, respectively. It is defined by the Equation (2):

$$(z_i^k)_N = \frac{z_i^k - z_{min}^k}{z_{max}^k - z_{min}^k} \tag{2}$$

Where k is the data set to be normalized, i is the set item, z_{max}^k is the upper limit of the data set, and z_{min}^k is the lower limit of the data set. After normalization it was obtained the database to be used for this study. The normalized sample database is given in **Table 1**.

Once the database is obtained, an ANN model could be built. Because of its nonlinearity in data, a multi-layer preceptor network was required. It does not contain cycles. Each layer can produce combinations of straight lines in order to form a convex region. One layer could form a convex region inside another convex region, formed by the former layer. In layered architectures normally all units from one layer are connected to all other units in the following layer [10]. It is depicted in **Figure 2**.

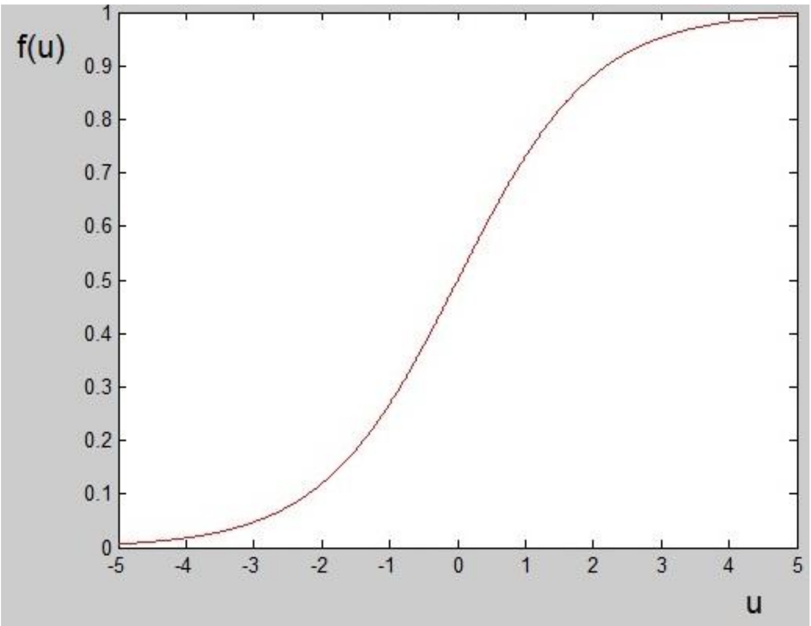

Figure 1: The Sigmoid function curve.

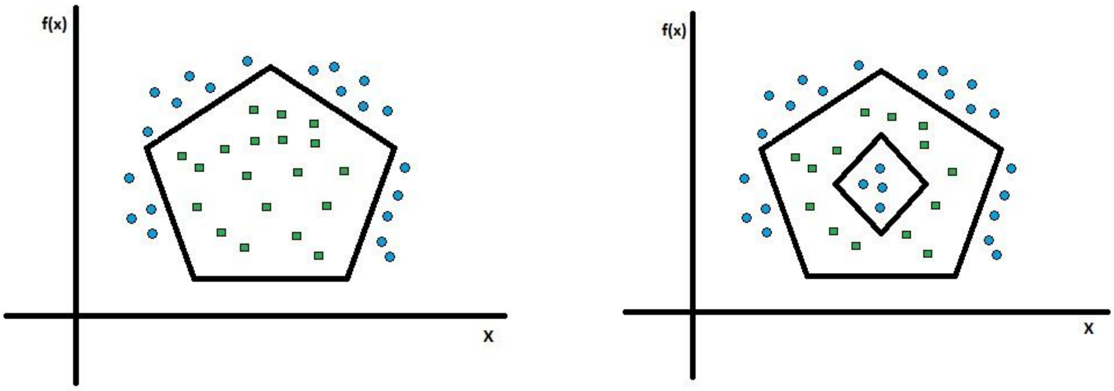

Figure 2: (a) Regions defined by the second hidden layer processing; (b) Regions defined by the output layer processing.

Table 1: Normalized database (IMPUT, OUTPUT).

f_{ck} (MPa)	Coarse aggregate			Portland cement			$MgSO_4$ solution (g/l)	$MgSO_4$ wet-dry cycle (days)	Time of travel of ultrasonic pulse wave	Compressive strength	Surface porosity
	CC	CD	GN	CPII	CPIII	CPIV					
20	1	0	0	1	0	0	0	90	0.469858156	0.161111111	0.082278481
20	1	0	0	1	0	0	10	28	0.572695035	0.077777778	0.286919831
20	1	0	0	1	0	0	50	180	0.909574468	0	0.474683544
20	1	0	0	0	1	0	0	180	0.310283688	0.211111111	0.08649789
20	1	0	0	0	1	0	10	90	0.446808511	0.35	0.116033755
20	1	0	0	0	1	0	50	28	0.427304965	0.272222222	0.219409283
20	1	0	0	0	0	1	0	28	0.184397163	0.083333333	0.464135021
20	1	0	0	0	0	1	10	180	0.59751773	0.077777778	0.128691983
20	1	0	0	0	0	1	50	90	0.666666667	0.122222222	0.162447257
20	0	1	0	1	0	0	0	28	0.356382979	0.061111111	0.314345992
20	0	1	0	1	0	0	10	180	0.377659574	0.044444444	0.35021097
20	0	1	0	1	0	0	50	90	0.508865248	0.083333333	0.734177215
20	0	1	0	0	1	0	0	90	0.184397163	0.283333333	0.033755274
20	0	1	0	0	1	0	10	28	0.292553191	0.022222222	0.191983122
20	0	1	0	0	1	0	50	180	0.416666667	0.033333333	0.449367089
20	0	1	0	0	0	1	0	180	0.331560284	0.005555556	0.723628692
20	0	1	0	0	0	1	10	90	0.484042553	0.15	0.14556962
20	0	1	0	0	0	1	50	28	0.432624113	0.038888889	0.276371308
20	0	0	1	1	0	0	0	180	0.65248227	0.133333333	0.284810127
20	0	0	1	1	0	0	10	90	0.757092199	0.294444444	0.345991561
20	0	0	1	1	0	0	50	28	1	0.1	0.443037975
20	0	0	1	0	1	0	0	28	0.556737589	0.294444444	0.175105485
20	0	0	1	0	1	0	10	180	0.656028369	0.316666667	0.217299578
20	0	0	1	0	1	0	50	90	0.787234043	0.483333333	0.234177215
20	0	0	1	0	0	1	0	90	0.673758865	0.138888889	1
20	0	0	1	0	0	1	10	28	0.624113475	0.133333333	0.29535865
20	0	0	1	0	0	1	50	180	0.895390071	0.077777778	0.227848101
50	1	0	0	1	0	0	0	90	0.19858156	0.572222222	0.187763713
50	1	0	0	1	0	0	10	28	0.721631206	0.527777778	0.251054852
50	1	0	0	1	0	0	50	180	0.207446809	0.7	0.356540084
50	1	0	0	0	1	0	0	180	0.274822695	0.794444444	0.075949367
50	1	0	0	0	1	0	10	90	0.161347518	0.627777778	0.198312236
50	1	0	0	0	1	0	50	28	0.473404255	0.538888889	0.265822785
50	1	0	0	0	0	1	0	28	0.411347518	0.6	0.196202532
50	1	0	0	0	0	1	10	180	0.29964539	0.894444444	0.056962025
50	1	0	0	0	0	1	50	90	0.276595745	0.683333333	0.088607595
50	0	1	0	1	0	0	0	28	0.29787234	0.588888889	0.390295359
50	0	1	0	1	0	0	10	180	0.093971631	0.583333333	0.191983122
50	0	1	0	1	0	0	50	90	0.028368794	0.4	0.588607595
50	0	1	0	0	1	0	0	90	0	0.733333333	0
50	0	1	0	0	1	0	10	28	0.413120567	0.488888889	0.303797468
50	0	1	0	0	1	0	50	180	0.24822695	0.666666667	0.713080169
50	0	1	0	0	0	1	0	180	0.138297872	0.75	0.194092827
50	0	1	0	0	0	1	10	90	0.120567376	0.527777778	0.116033755
50	0	1	0	0	0	1	50	28	0.413120567	0.466666667	0.377637131
50	0	0	1	1	0	0	0	180	0.390070922	1	0.025316456
50	0	0	1	1	0	0	10	90	0.404255319	0.627777778	0.278481013
50	0	0	1	1	0	0	50	28	0.934397163	0.8	0.400843882
50	0	0	1	0	1	0	0	28	0.842198582	0.827777778	0.156118143
50	0	0	1	0	1	0	10	180	0.478723404	0.877777778	0.132911392
50	0	0	1	0	1	0	50	90	0.457446809	0.705555556	0.206751055
50	0	0	1	0	0	1	0	90	0.384751773	0.705555556	0.206751055
50	0	0	1	0	0	1	10	28	0.930851064	0.727777778	0.202531646
50	0	0	1	0	0	1	50	180	0.546099291	0.944444444	0.291139241

The network used in this study consists of an imput layer with 54 nodes, a hidden layer with 5 nodes, and a one-nodded output layer. The number of hidden layers is considered equal to one in order to improve the efficiency and compatibility of the model in predicting and testing the accuracy of the new experimental datasets faster and more easily [11]. The architectural layout of the backpropagation network is presented in **Figure 3**.

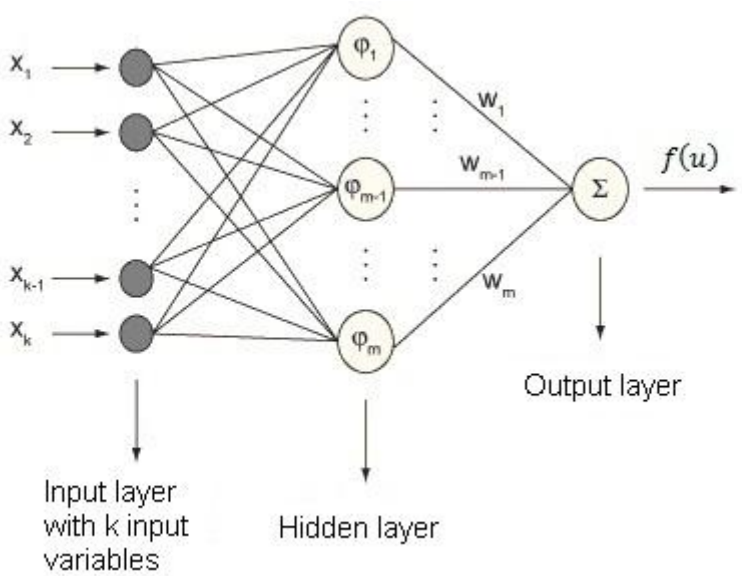

Figure 3: Architectural layout of neural network model, with *k* ranging from 1 to 54, *m* ranging from 1 to 5, and $f(u) = \frac{1}{1+e^{-\beta u}}$.

The performance results of the ANN model are plotted in **Figures 4, 5 and 6** for the 43rd database sample simulation. In these figures the time index goes on the x-axis, and the total error (the sum of squared differences between the predicted value data and the measured experimental data) goes on the y-axis; the red line is the training error, and the blue line is the testing error. It is concluded from the **Figures 4, 5 and 6** that Portland cement concrete degradation by sulphate exposure is accurately modeled by ANN. The ANN model showed good correlation between predicted and experimental test values, making sure the architecture network is accurate.

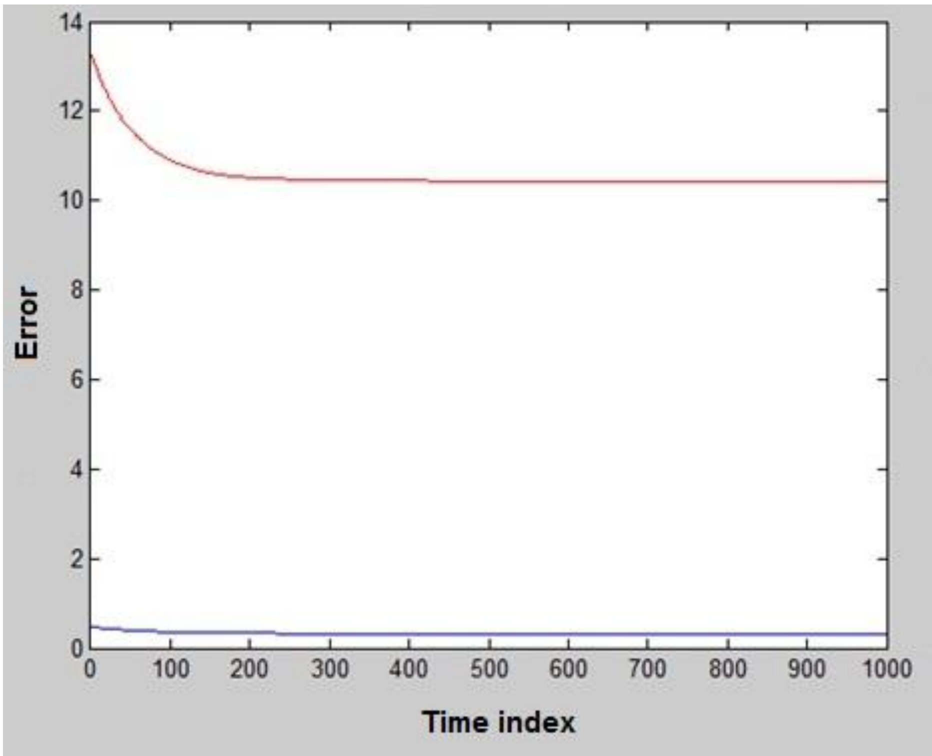

Figure 4: Error figure for the 43rd database sample simulation of time of travel of ultrasonic pulse wave. Red line: training error. Blue line: testing error.

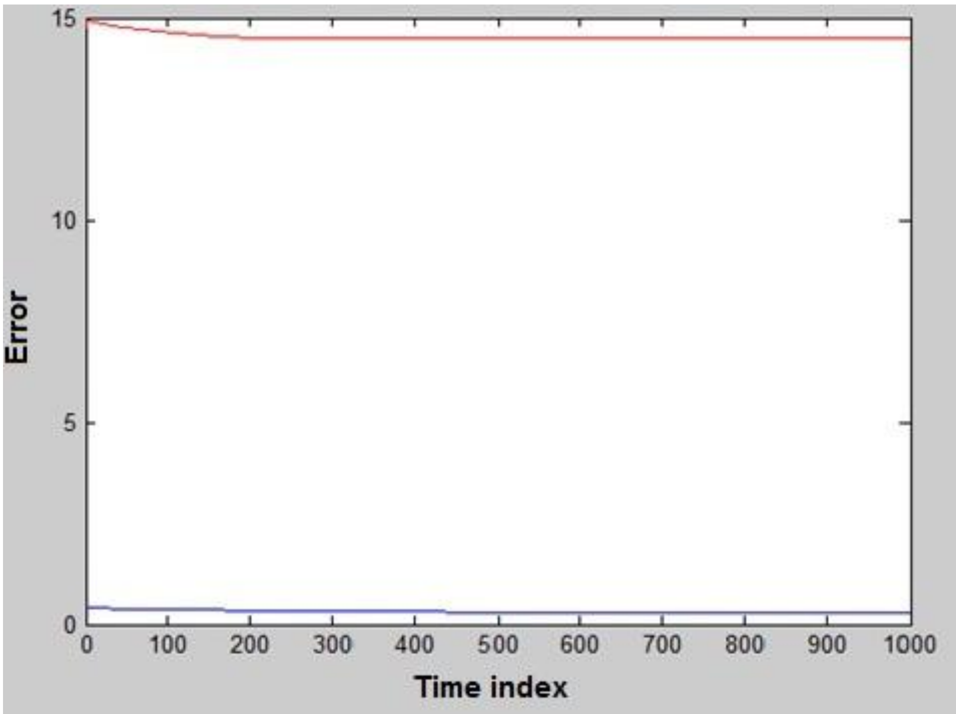

Figure 5: Error figure for the 43rd database sample simulation of compressive strength. Red line: training error. Blue line: testing error.

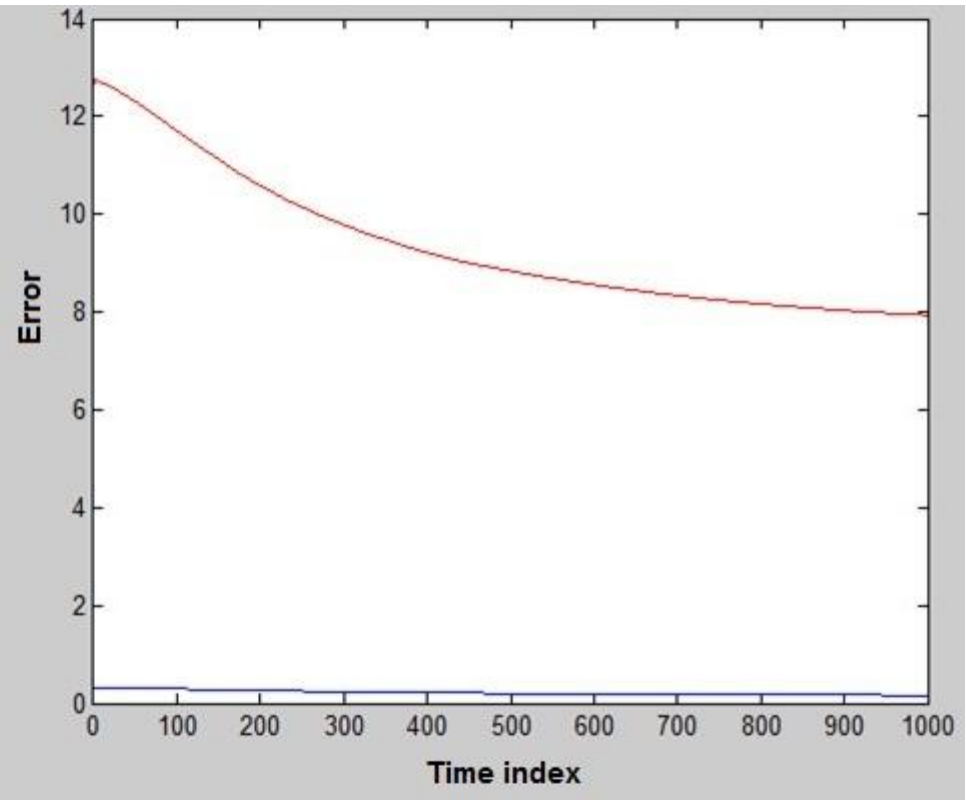

Figure 6: Error figure for the 43rd database sample simulation of surface porosity. Red line: training error. Blue line: testing error.

4. CONCLUSIONS

The present work presented the application of neural network to evaluate Portland cement concrete degradation by sulphate exposure. An ANN model was developed, trained and tested. It was observed that the ANN actually learned the nonlinear deviation curve belonging experimental database.

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