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Predicting Density and Compressive Strength of Concrete Cement Paste Containing Silica Fume Using Artificial Neural Networks

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Abstract. *Artificial Neural Networks (ANNs) have recently been introduced as an efficient artificial intelligence modeling technique for applications involving a large number of variables, especially with highly nonlinear and complex interactions among input/output variables in a system without any prior knowledge about the nature of these interactions. Various types of ANN models are developed and used for different problems. In this paper, an artificial neural network of the feed-forward back-propagation type has been applied for the prediction of density and compressive strength properties of the cement paste portion of concrete mixtures. The mechanical properties of concrete are highly influenced by the density and compressive strength of concrete cement paste. Due to the complex non-linear effect of silica fume on concrete cement paste, the ANN model is used to predict density and compressive strength parameters. The density and compressive strength of concrete cement paste are affected by several parameters, viz, water-cementitious materials ratio, silica fume unit contents, percentage of super-plasticizer, curing, cement type, etc. The 28-day compressive strength and Saturated Surface Dry (SSD) density values are considered as the aim of the prediction. A total of 600 specimens were selected. The system was trained and validated using 350 training pairs chosen randomly from the data set and tested using the remaining 250 pairs. Results indicate that the density and compressive strength of concrete cement paste can be predicted much more accurately using the ANN method compared to existing conventional methods, such as traditional regression analysis, statistical methods, etc.*

Keywords: *Cement paste; Compressive strength; Density; Neural network; Silica fume.*

INTRODUCTION

Concrete has been used as a construction material for more than a century. During this period of time, concrete has undergone a continuous development, e.g. the growing use of secondary cementitious materials in the binding phase. The use of binder admixtures in the production of concrete with enhanced performance (also known as High Performance Concrete or simply HPC) has received a great amount of attention recently. One of the most important binder admixtures to offer a significant contribution to HPC production is silica fume, a pozzolanic material [1,2].

Concrete, as a non-homogeneous material, consists of separate phases; hydrated cement paste, transition zone and aggregate. Although most of the characteristics of concrete are associated with the average characteristics of a component microstructure, the compressive strength and failure of concrete are related to the weakest part of the microstructure. Cement paste properties are of great significance in concrete technology. The compressive strength of cement paste is mainly related to Van der Walls forces. Therefore, the more compacted the concrete, the higher is the compressive strength. One porosity reducing factor is the water-cement ratio and the other factor that affects concrete porosity is filler materials, such as silica fume [1,2].

In recent years, ANNs have shown exceptional performance as regression tools, especially when used

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for pattern recognition and function estimation. They can capture highly non-linear and complex relations among input/output variables in a system without any prior knowledge about the nature of these interactions. Unlike traditional parametric models, these models are able to construct a supposedly complex relationship between input and output variables with an excellent level of accuracy compared with that of conventional methods [3]. The main advantage of ANNs is that one does not have to assume an explicit model form, which is a prerequisite in the parametric approaches. Indeed, in ANN models, a relationship of a possibly complicated nature between input and output variables is generated by the data points. In comparison to parametric methods, ANNs can deal with relatively imprecise or incomplete data and approximate results, and are less vulnerable to outliers. They are highly parallel, that is, their numerous independent operations can be executed simultaneously [4].

Basma et al. [5] proposed a method for the prediction of cement degree of hydration using ANN. The results indicated that the ANNs are very efficient in predicting the concrete degree of hydration with great accuracy using minimal processing data. Nehdi et al. [6] applied a neural network model for performed-foam cellular concrete. Results showed that the production yield, foamed density, unfoamed density and the compressive strength of cellular concrete mixtures can be predicted much more accurately using the ANN method compared to existing parametric methods. Jespen [7] designed a neural network to investigate the influence of different parameters on the salt frost resistance of concrete. Ju-Won Oh et al. [8] developed an ANN model for the proportioning of concrete mixtures. Nehdi et al. [9] used an ANN model for predicting the performance of self-compacting concrete mixtures. Zong, Gung and Yun [10] utilized an automatic knowledge acquisition system, based on neural networks, to design concrete mixtures. In a later work, Gung and Zong [11] proposed a method to predict 28-day compressive strength by using multi layer feed forward neural networks. Lai and Serra [12] developed a model, based on neuro computing, for prediction of the compressive strength of cement conglomerates. Yeh [13] developed a strength based Artificial Neural Network (ANN) model, which was found to be more accurate than the one based on regression analysis. It was also discovered that his ANN model gave the detailed effects of the proportions of each variable from the concrete mixtures. Dias and Pooliyadda [14] used back propagation neural network models to predict the strength and slump of ready mixed ordinary concrete and high strength concrete, in which chemical admixtures were used.

Attempts have been made in the past to devise a kinetic model for cement paste properties to predict the phenomena occurring in concrete, but the focus of these models has been on predicting density, compressive strength, deformation under loading, the cracking of sufficiently hardened concrete and etc. The models have not yet reached the stage where they can explain the changes in the physical properties of the cement paste portion of the concrete [5-14].

Predicting the properties of cement paste is of great significance and difficult to achieve as a function of the mixture gradient and physical properties of concrete, hence, a nonlinear prediction model needs to be considered. The uncertainties associated with the parameters affecting the density and compressive strength of cement paste make it difficult to exactly estimate such properties [1,4]. Knowing the properties of cement paste, a better understanding of concrete performance properties can be taken into account [1,2]. Considering the influence of silica fume on the transition zone and cement paste and the complex and nonlinear effect of silica fume on concrete cement paste, a set of experiments were carried out on cement paste with different water-cementitious materials and silica fume unit contents, in order to investigate the effect of silica fume on cement paste. An ANN model is then developed, based on the data produced, to predict density and compressive strength parameters.

NEURAL NETWORKS

ANN modeling, a paradigm for computation and knowledge representation, is originally inspired by the understanding and abstraction of the biological structure of neurons and the internal operation of the human brain. A neural network is a network of many simple processors that are called nodes. A multilayer perceptron may be thought of as consisting of layers of parallel data processing cells. Each node (neuron) has a small amount of local memory. Nodes in the input layer only act as buffers for distributing the input signals to nodes in the hidden layer. The nodes are connected by connections; each usually carrying numeric data called weights, encoded by any of the existing methods. Each node in the hidden layer sums up its input signals after weighting them with the strengths of the respective connections from the input layer and computes its output as a function of the sum. The nodes operate only on the local data and on the inputs they receive via the connections. The differences between the computed output and the target are combined together by an error function to give the network the verification set, and used to keep an independent check of the progress of the algorithm. Training of the neural network is stopped when the error for the verification set begins to increase [3,4,8].

The main principle of neural computing is the decomposition of the input-output relationship into a series of linearly separable steps using hidden layers [4]. There are three distinct steps in developing an ANN-based solution:

1. Data transformation or scaling;
2. Network architecture definition, where the number of hidden layers, the number of nodes in each layer and the connectivity between the nodes are set;
3. Construction of a learning algorithm in order to train the network [3,6].

Figure 1 shows the simple architecture of a typical network that consists of an input layer, hidden layers, an output layer and connections between them. Nodes in the input layer represent possible influential factors that affect the network outputs and have no computation activities, while the output layer contains one or more nodes that produce the network output. Hidden layers may contain a large number of hidden processing nodes. A feed-forward back-propagation network propagates the information from the input layer to the output layer, compares the network outputs with known targets and propagates the error from the output layer back to the input layer, using a learning mechanism to adjust the weights and biases [3,8].

In general, the net input to each node is calculated as:

$$N_j^l = \sum_{i=1}^{n} W_{ji}^l . X_i^{l-1} + \beta_j^l, \tag{1}$$

where W_{ji}^l is the weight that connects node j in layer l to node i in layer $l-1$; n is the number of nodes in layer $l-1$; β_j^l is a threshold value assigned to node j in layer l; and X_i^{l-1} is the input coming from node i in layer $l-1$ to node j in layer l. The net input, N_j^l, is then modified by an activation function, f, to generate an output value, Y_j^l, given by:

$$Y_j^l = f(N_j^l), \tag{2}$$

where f is a nonlinear activation function assigned to each node in the network. The learning mechanism of this back-propagation network is a generalized delta rule that performs a gradient-descent on the error space, in order to minimize the total error between the calculated and desired values at the output layer during modification of the connection weights. The implementation of this algorithm updates the network weights and biases in the direction in which the error decreases most rapidly. Training is accomplished in an iterative manner. Each iteration cycle involves the feed-forward computation followed by an error-backward propagation to modify the connection weights. Convergence depends on the number of hidden layer nodes, learning rate parameters and the size of the data set required to create the proper results. Furthermore, there is no structured algorithm to obtain the optimal structure and parameters of neural networks; therefore, one should find the optimal network by trial and error. The most interesting property of a network is its ability to generalize new cases. For this purpose, an independent data set is used to test the neural network and check its performance. When verification and test errors are reasonably close together, the network is likely to generalize well [3,8].

Upon successful completion of the training process, a well-trained neural network is not only capable of computing the expected outputs of any input set of data used in the training stage, but should also be able to predict, with an acceptable degree of accuracy, the outcome of any unfamiliar set of input located within the range of the training data [3,6].

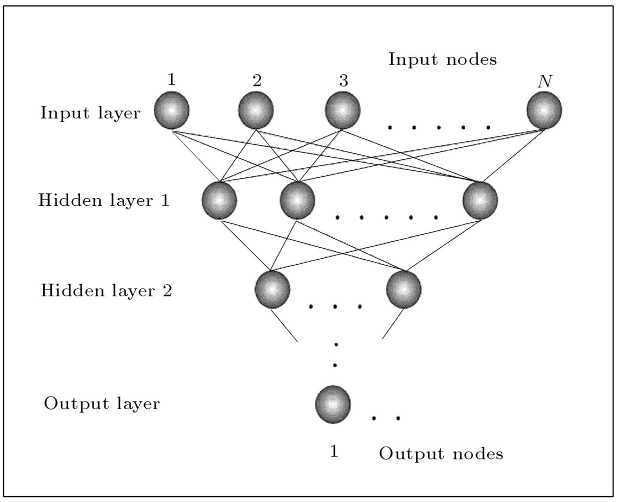

Figure 1. Neural network design topology.

SELECTION OF DATABASE

The selection of the database chosen to train a neural network such that it will be capable of capturing the relationships between the parameters of the cement paste mixtures and its mechanical properties, density and compressive strength, is of great importance. It must be trained on large and comprehensive sets of reliable experimental data that contain influential factors regarding cement paste density and compressive strength [9].

The data set for neural network analysis was a subset from the database of a cement paste containing silica fume mixture properties [15]. The density and compressive strength were measured in the laboratory by preparing several mixtures of cement paste. In this study, cement, silica fume, water and super plasticizer were used for the production of these mixtures. Two

Table 1. Range, average and standard deviation of measured input and output variables.

Variables	Range	Average	Standard Deviation
Water-cementitious materials ratio (W/cm)	0.35 to 0.65	0.57	0.05
Cement (kg/m^3)	430 to 1140	802.3	106.8
Silica fume (kg.m^3)	75 to 625	290	87.13
Super-plasticizer (kg/m^3)	0 to 25	2.5	1.88
Cement type	1 and 2	-	-
Density (kg/m^3)	1600 to 2100	1715.4	59.36
Compressive strength (MPa)	15 to 65	36	8.02

types of cement (Type I and Type II) with the W/cm of 0.35 to 0.65 and silica fume unit contents of 75 kg/m^3 to 625 kg/m^3 were used to prepare the specimens. All the specimens were cured for 28 days at an average temperature of 20°C. This led to the development of a large number of data sets. Table 1 shows the ranges, average values and standard deviation of all relevant parameters. A detailed examination of the data in the database showed that many were missing the information necessary for the neural network analysis. Ultimately, a total of 600 data pairs have, therefore, been selected from the experimental database, as stated earlier.

NEURAL NETWORK ARCHITECTURE

There is no effective procedure for identifying the optimal architecture of a network before training. However, it is important for the hidden layers to have a small number of nodes. An excessive number of hidden nodes may cause the network to memorize the training data. In such cases, the ANN would not be able to interpolate effectively between adjacent training data points. Too few hidden nodes, on the other hand, will limit the network's ability to construct an adequate relationship between input and output variables [3].

The number of hidden layers and nodes are usually determined via a trial and error procedure. There are some rules to estimate the number of hidden nodes. According to the method suggested by Dave Anderson and George McNeill [3], an upper bound for the number of processing nodes in the hidden layers can be calculated by dividing the number of input-output pairs in the training set by the total number of input and output nodes in the network, multiplied by a scaling factor between five and ten. Larger scaling factors are used for relatively noisy data.

The water-cementitious materials ratio (W/cm), the unit contents of the cement, the silica fume and super plasticizer and cement type parameters are represented by the input nodes, while the output layer contains two nodes representing density and compressive strength. Following the guidelines suggested by Dave Anderson and George McNeill [3] and some preliminary computations, a network architecture containing two hidden layers was adopted. The first hidden layer included five nodes, while the second hidden layer had only three nodes and a full connection between the nodes in the adjacent layers was selected. The network architecture can be seen schematically in Figure 2. The assignment of transfer functions and the number of nodes are also shown in Table 2. A free access ANN package (Qnet) of the feed-forward back-propagation type was used in this study [16].

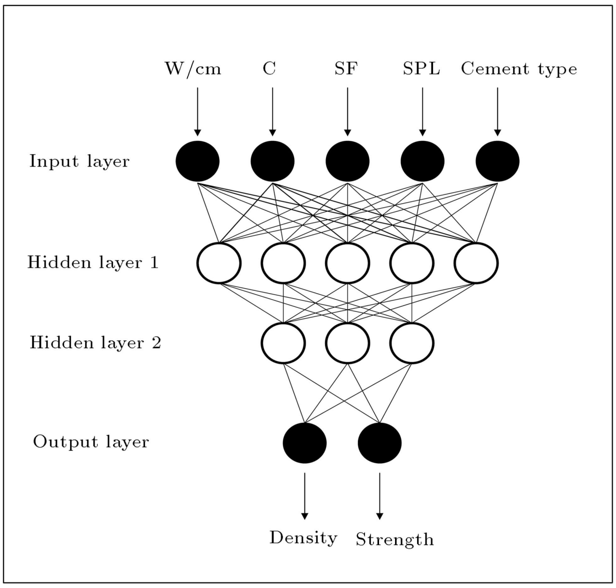

Figure 2. Architecture of neural network model.

Table 2. Network information.

Layer	Number of Nodes	Transfer Function
Input layer	5	Linear
Hidden layer 1	5	Gaussian
Hidden layer 2	3	Tanh
Output layer	2	Sigmoid

TRAINING OF ANN MODEL

The training procedure was carried out by presenting the network with the set of experimental data in a patterned format. Each training pattern includes an input set of five parameters representing the cement paste mixture ingredients (that is, W/cm, C, SF, SPL, cement type) and a corresponding output set representing the cement paste properties (that is, density and compressive strength). The network is presented with the variables in the input vector of the first training pattern, followed by an appropriate computation through the nodes in the hidden layers and prediction of the appropriate outputs. The error between the predicted output and target value is calculated and stored. The network is then presented with the second training pattern and so on until the network has gone through all the data available for training the network. The Root-Mean-Square (RMS) of the error is then calculated and back propagated to the network. Biases and weights or the connection strength between nodes are modified during the back propagation phase such that the (RMS) errors are reduced. The process of the introduction of training input-output pairs to the network, calculation of the (RMS) error and, finally, the adjustment of weights and biases to reduce the (RMS) error are referred to as one iteration. This process continues until convergence is achieved or the maximum number of iterations is reached [3,6]. The trained ANN model is represented by the connection weights once the above procedure is converged. This process is illustrated in Figure 3.

To avoid the over-fitting of the neural network model to the data during iterative training, a separate set of the data set was used to validate the model at some intervals during training. Training is stopped when the error for the validation set begins to increase. The network was trained and validated, based on 350 training patterns chosen randomly from the 600 available data sets. The remaining 250 pairs of independent data were used to test the network after completion of training and validation in order to assess its performance on data to which it has never before been exposed. The training process and the associated ANNs analyses were carried out with an optimal value of learning rate of 0.0035 and maximum number of iterations of 20000 with an error goal of 0.000.

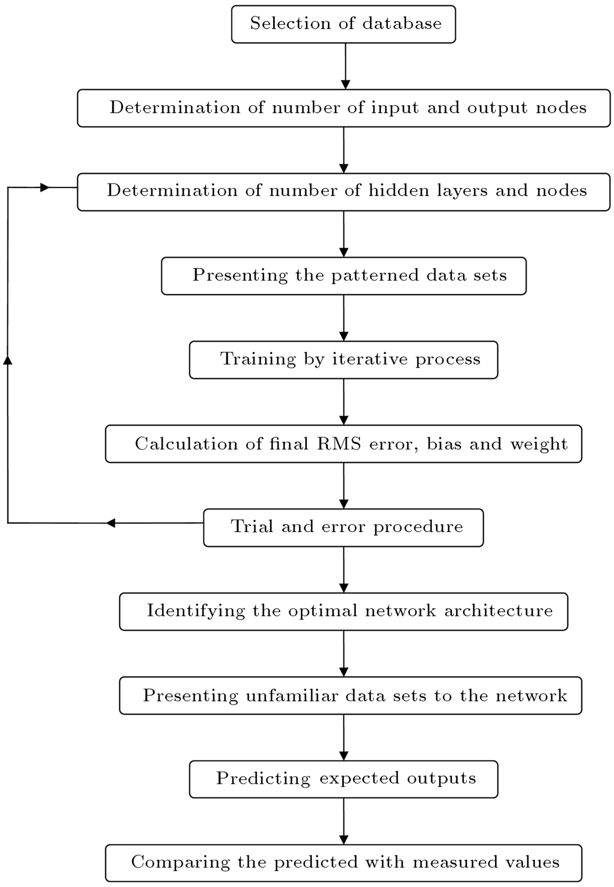

Figure 3. Processing neural network model.

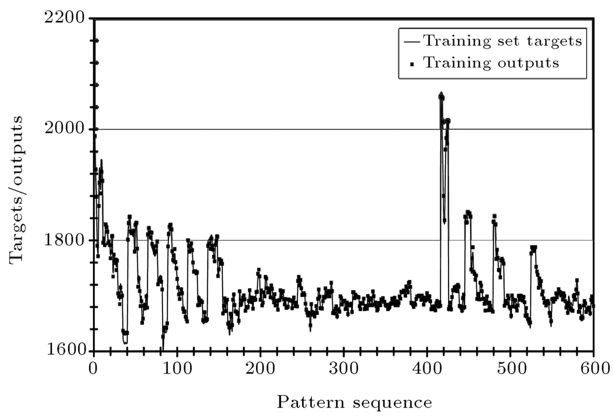

Figure 4a. Targets/outputs vs pattern sequence (node 1).

RESULTS AND DISCUSSION

The network was trained to predict cement paste properties (density and compressive strength) using a total of 350 training and validating data sets and 250 testing data sets. Figures 4a and 4b compare the output and target values of the density and compressive strength of cement paste for all the 600 available data sets. Table 3 shows the training information and Figures 5a and 5b show the convergence characteristics of the ANN model during the training and testing phases, respectively. The correlation histories are also shown in Figures 6a and 6b for the training and testing stages. It is clearly seen that correlation is very high in the early stages of the training process, but gradually becomes slower in later iterations.

Figure 7 illustrates the distribution of the network outputs vs the target values for the training data

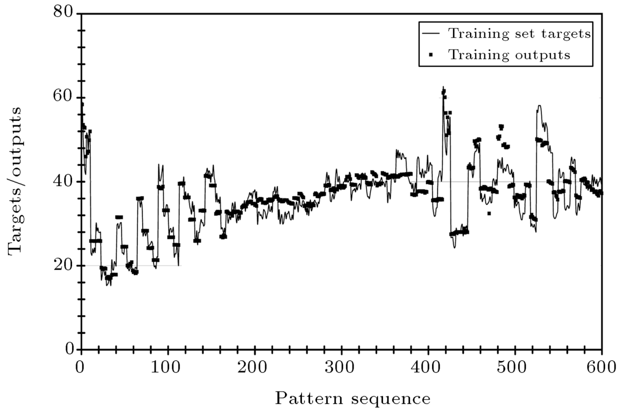

Figure 4b. Targets/outputs vs pattern sequence (node 2).

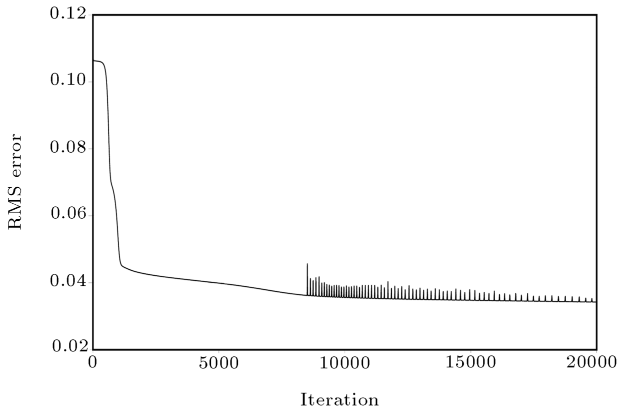

Figure 5a. Training RMS error history vs iteration.

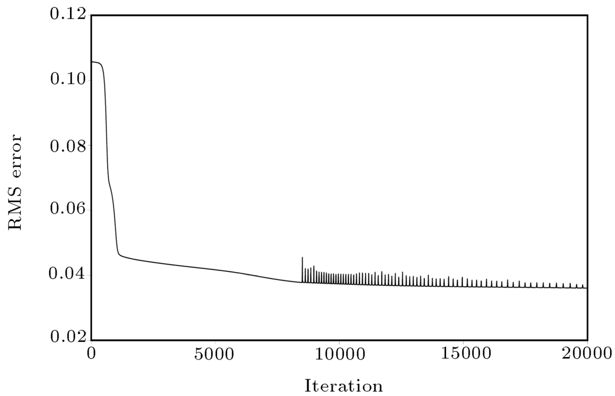

Figure 5b. Testing RMS error history vs iteration.

sets. All data points are distributed along the optimal agreement line, with the training and testing Root-Mean-Square (RMS) errors of 0.034385 and 0.034780, respectively. The final biases and absolute maximum errors and correlation for output nodes are also listed in Table 4. The correlation between predicted and measured compressive strength is seen to be satisfactory. It is generally lower for density, especially at higher compressive strength values. In practice, the compressive strength results of the cement paste mixture exhibit high variability between batches affected by the mixing technique, consolidation, temperature, curing and the testing method. The relatively larger prediction error and less correlation compressive strength may, therefore, be associated to high variability in the mixture development rather than the prediction method.

To test the accuracy of the ANN model, the final trained model was called upon to recall the data not used in the training process. A total of 20 cement

Table 3. Training information.

Iterations	20000
Training RMS Error*	0.034385
Testing RMS Error*	0.034780
Learn Rate	0.003500

* The sum of squared differences between the network targets and actual outputs for a given input vector or set of vectors (root-mean-square error).

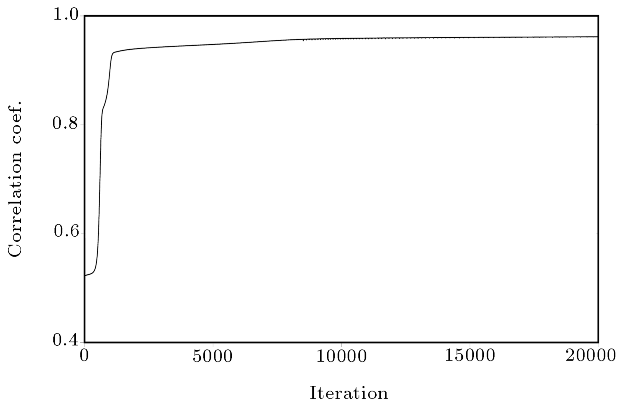

Figure 6a. Training correlation history vs iteration.

Table 4. Biases, max errors and correlations for output layer.

Node	Bias*		Max Error		Correlation	
	Training Data	**Test Data**	**Training Data**	**Test Data**	**Training Data**	**Test Data**
1	0.6651	-0.2158	22.46985	32.76013	0.99723	0.99469
2	0.0312	-0.0285	5.51261	4.77564	0.91853	0.90763

* A node parameter that is summed with the node's weighted inputs and passed through the node's transfer function to generate the node's output.

Table 5. Measured and predicted values of outputs variables for data sets used in testing of ANN model.

No.	Testing Data Sets					Density (kg/m^3)		Compressive Strength (MPa)	
	Water-Cementitious Materials Ratio	Cement (kg/m^3)	Silica Fume (kg/m^3)	Super Plasticizer (kg/m^3)	Cement Type	Measured	Predicted	Measured	Predicted
1	0.37	926.280	463.140	11.115	2	1914.62	1930.00	50.38	51.62
2	0.4	934.800	420.660	9.348	2	1906.99	1908.75	50.38	50.61
3	0.42	923.163	387.729	7.385	2	1868.85	1866.26	51.54	49.42
4	0.45	1020.558	306.168	6.123	2	1929.88	1922.62	50.76	49.99
5	0.5	1117.818	78.247	0.000	2	1794.10	1793.34	24.03	25.70
6	0.5	1026.040	174.427	1.026	2	1801.73	1806.62	33.97	33.92
7	0.55	762.036	320.055	3.201	2	1680.44	1679.53	39.00	41.36
8	0.55	1062.902	75.403	0.000	2	1762.82	1756.40	18.99	20.29
9	0.57	780.843	304.529	2.343	2	1706.38	1704.96	34.49	37.44
10	0.58	768.702	292.107	2.075	2	1678.15	1678.54	32.41	34.90
11	0.6	942.854	113.143	0.000	2	1689.59	1684.68	19.38	19.60
12	0.65	746.887	261.411	1.494	2	1665.19	1671.75	27.51	29.38
13	0.35	1078.299	431.320	21.566	1	2049.55	2016.79	62.39	59.11
14	0.4	913.335	456.667	11.873	1	1929.88	1959.84	50.76	52.98
15	0.45	936.546	421.446	6.556	1	1975.64	1952.66	51.54	51.45
16	0.5	916.808	302.547	0.917	1	1829.95	1844.31	44.37	43.32
17	0.55	789.731	355.379	3.159	1	1778.08	1784.68	47.28	47.80
18	0.6	731.917	329.363	1.464	1	1699.51	1698.11	35.30	37.28
19	0.62	665.399	365.970	1.996	1	1672.81	1673.76	38.90	36.39
20	0.65	845.297	194.418	0.000	1	1715.53	1707.36	29.45	27.26

paste mixtures, unfamiliar to the network in the range of training data sets, were presented to the ANN model and the network was required to predict the density and compressive strength associated with each mixture. The mixture proportion and the measured and predicted values are listed in Table 5.

As mentioned previously, a set of experimental data, including 600 pairs of data, was used in this study, from which 350 training and validating patterns were chosen arbitrarily and the remaining 250 pairs were used as measured data, to test and verify the efficiency and validity of the predicted values by the network. A good agreement between the measured and predicted values of the density and compressive

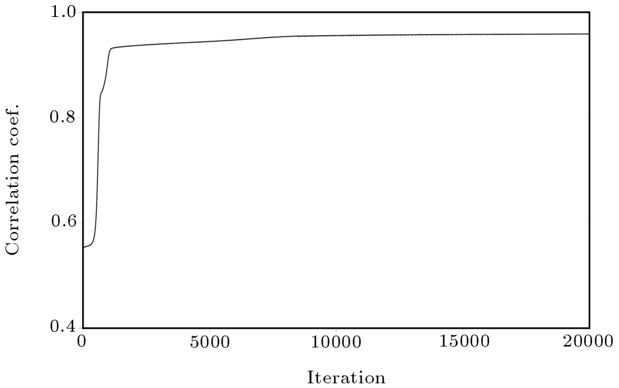

Figure 6b. Testing correlation history vs iteration.

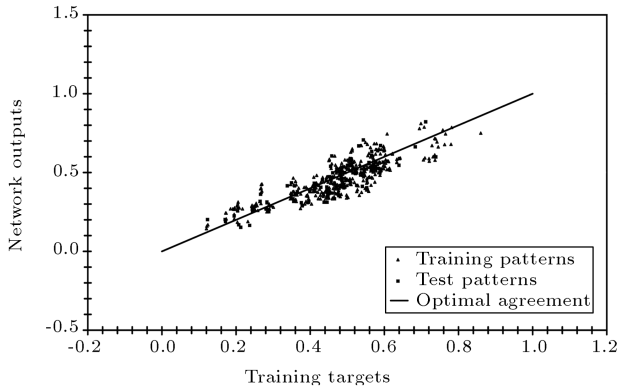

Figure 7. Net outputs vs targets.

strength is observed, as shown in Figure 8a and 8b. It can be, therefore, concluded that the proposed ANN model is adequately able to predict the above mentioned properties of cement paste.

Effect of Silica Fume and Its Optimum Content on Concrete Cement Paste

Figures 9a and 9b show the color contour of density and compressive strength vs unit content of Silica Fume (SF) and water cementitious materials ratio (W/cm). It is generally believed that there exists an optimum content of silica fume, at which the density and compressive strength are maximum. Therefore, several sets of data, each containing 23 data, were arbitrarily created, with constant values of W/cm presented to the ANN model, and the network was called upon to predict the corresponding density and compressive strength.

The variation of density and compressive strength, with the silica fume unit content value for three of these sets, with W/cm values of 0.47, 0.54 and 0.61, is plotted and shown in Figures 10a and

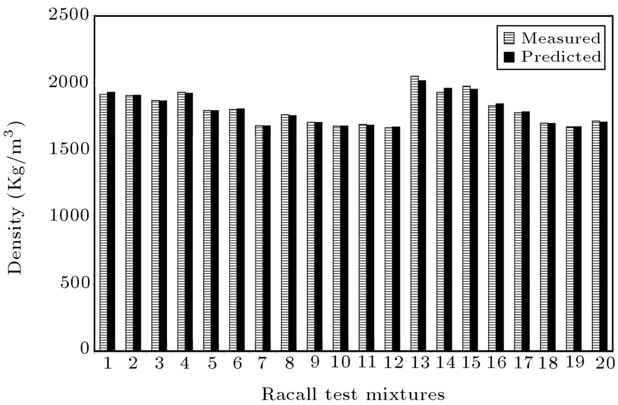

Figure 8a. Performance of ANN model predictions for cement paste density.

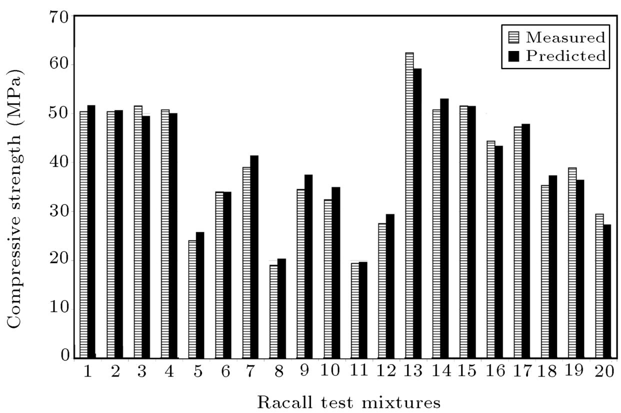

Figure 8b. Performance of ANN model predictions for cement paste compressive strength.

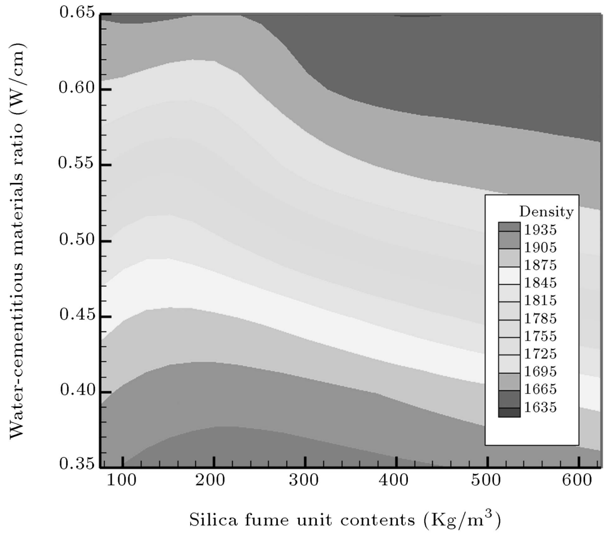

Figure 9a. Output node 1 vs input node 1 and input node 3.

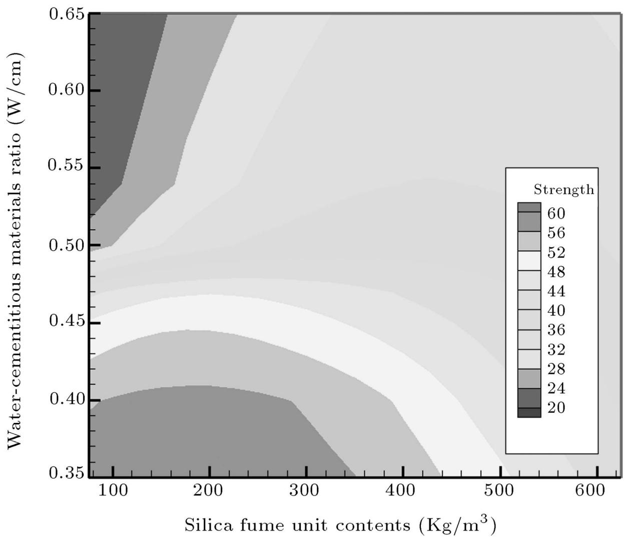

Figure 9b. Output node 2 vs input node 1 and input node 3.

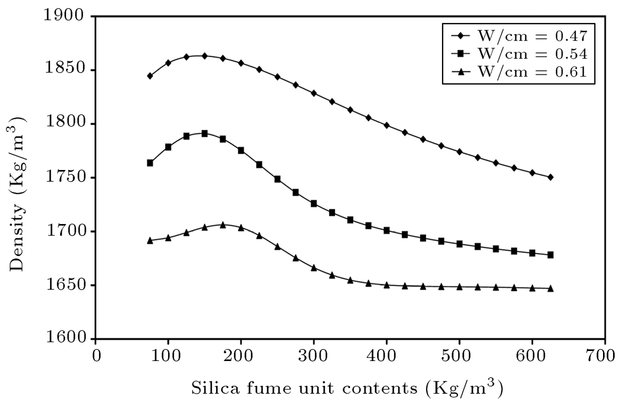

Figure 10a. Density vs silica fume unit contents at different constant W/cm.

10b. The existence of an optimum content of silica fume in the cement paste is clearly verified. It is also shown that this optimum is not constant but depends on the W/cm of the mixture. It is also noted that, for each value of W/cm, the maximum density occurs at a silica fume unit content value different from that resulting in maximum compressive strength. This difference can be contributed to the way in which the silica fume affects the density and compressive strength of the mixture. Silica fume content affects the compressive strength characteristics of the mixture through chemical pozzolanic activity and physical micro filler action, while its influence on the density is limited to physical filler action. The optimum content of silica fume for maximum density and compressive strength is seen, from Figures 10a and 10b, to be in the range of approximately 125 kg/m^3 to 200 kg/m^3 and 225 kg/m^3 to 475 kg/m^3, respectively. This conclusion can, of course, only be drawn for the data used in this experimentation.

Bhanja and Sengupta [17] have investigated the effects of silica fume and reported similar observations, indicating that both the pozzolanic and filler effects of silica are highly significant. Considering the differences between the optimum silica fume content for density and compressive strength, it can be concluded that the role of silica fume in maximizing the cement paste compressive strength is twofold, namely; filler effect and pozzolanic effect. Some researchers, however, contradict these conclusions. A. Bentur and K.L. Scrivener [18] have an opposite report. Papadakis [19] has reported that the silica fume added in excess of that required for pozzolanic action is inert and, thus, not necessary. Goldman [20,21] and Bhanja and Sengupta [17] have reported that the amount of silica fume contributing to the physical effect is comparable to, or even more significant than, the amount contributing to the pozzolanic effect. Based on chemical considerations, Cohen has concluded that the highest

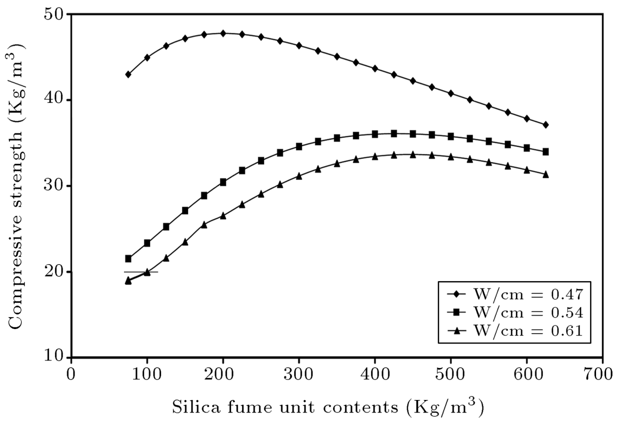

Figure 10b. Compressive strength vs silica fume unit contents at different constant W/cm.

strengths can be obtained with a 30 to 40% weight of silica fume. Wild, Sabir and Khatib [22] reported that the 28-day strength of silica fume concrete increased continuously up to a 16% replacement level, thereafter decreased and, again, increased, reaching maximum value at 28%, at a constant W/cm of 0.35.

It is worth mentioning that the proposed ANN model can be adjusted to include the effect of additional parameters, given the availability of sufficient data to train the network for the effects of these additional parameters. The number of input variables and the architecture of the network can be modified to include new mixture components. Hence, it is recommended to extend this model, once a more comprehensive database encompassing the effects of such parameters is available.

CONCLUSIONS

This paper presents a nontraditional approach to the prediction of the density and compressive strength of a cement paste mixture, based on ANN technology. Based on the findings of this investigation, the following conclusions can be drawn:

1. The proposed model demonstrates the ability of a feed-forward back-propagation neural network to predict the properties of the cement paste portion of concrete with sufficient accuracy. The model performed quite well in predicting, not only the density and compressive strength properties of cement paste mixtures used in the training process, but also those of test mixtures that were unfamiliar to the neural network.

2. Predicting the properties of cement paste as a function of the mixture ingredient, using analytical and traditional methods, is difficult to achieve, whereas a trained neural network model can predict such properties easily and accurately. Therefore, ANN can provide a drastically powerful alternative approach.

3. Although the prediction capability of any ANN model is limited to data located within the boundaries of the training range, the proposed model can be retrained to include a wider range of input variables by providing additional training sets covering the new range;

4. The existence of the optimum content of silica fume was well illustrated. It was also concluded that the optimum content of silica fume increases with increasing the value of the water-cementitious materials ratio, while the corresponding compressive strength decreases.

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