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Full Length Research Paper

Prediction of mechanical properties of cement containing class C fly ash by using artificial neural network and regression technique

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The aim of this study is to investigate the estimation ability of the effects of utilizing different amount of the class C fly ash on the mechanical properties of cement using artificial neural network and regression methods. For this reason, 0, 5, 10, 15 and 20% amount of the class C fly ash were substituted with cement and 40 x 40 x 160 mm dimension specimens were prepared. On the prepared specimens unit weight, flexural tensile strength and compressive strength tests were performed after the 2, 7 and the 28th days. 2 different estimation models regression techniques (RT) and the artificial neural network (ANN) methods were used for determining the flexural tensile strength and the compressive strength of the cement specimens. Experimental results were used in the estimation methods. Fly ash content (%), age of specimen (day) and unit weight (g/cm^3) were used as input parameters and flexural tensile and compressive strengths (N/mm^2) were used as output parameters. The developed models and the experimental results were compared in the testing data set. As a result, compressive and flexural tensile strength values of mortars containing various amounts class C fly ash can be predicted in a quite short period of time with tiny error rates by using the multilayer feed-forward neural network models than regression techniques.

Key words: Fly ash, cement, flexural tensile strength, compressive strength, regression, ANN.

INTRODUCTION

In view of the global sustainable development, it is imperative that supplementary cementing materials be used in replace of cement in the concrete industry. The most worldwide available supplementary cementing materials are silica fume (SF), a by-product of silicon metal and fly ash (FA), a by-product of thermal powder stations, and blast-furnace slag (BS), a byproduct of steel mill. It is estimated that approximately 600 million tons of FA are available worldwide now, but at present, the current worldwide utilization rate of FA in concrete is about 10% (Malhotra and Mehta, 2002). However, the recent development of green high performance concrete (GHPC) brings the abundant utilization of these mineral mixtures. When these different reactive mineral admix-tures are added into concrete at the same time, they develop their own characteristics with the development. SF can increase the strength of the concrete significantly; however, it affects the workability of the fresh concrete greatly, while adding large amount of FA to the concrete contributes the workability of the concrete but not to the strength. In addition, those mineral admixtures show different effects on the strength of the concrete within different ages due to their different pozzolan reactions (Chen and Liu, 2008). Mineral admixtures (MA) have been used in order to increase strength and improve durability and flowability of cementitious material. Blast furnace slag (BFS), fly ash (FA) and silica fume (SF) are typical mineral admixtures for achieving these properties. These minerals significantly affect rheology of cementitious material in the fresh state, which is directly related with developing strength, durability and engineering properties of hardened structures (Park et al., 2005).

The artificial neural networks solve very complex problems with the help of interconnected computing elements. Basically, the processing elements of a neural network are similar to the neurons in the brain, which consist of many simple computational elements arranged in layers (Raghu et al., 2009).

Neural networks became popular in the late 1980s and more recently, in the 1990s. Compared to traditional statistical methods, neural network analysis has been found to be very useful in diverse, real-world applications. An ANN can be defined as a data processing system consisting of a large number of simple, highly inter-connected processing elements (artificial neurons) in an architecture inspired by the structure of the cerebral cortex of the brain (Tantawy, 2009).

In the last years, artificial neural networks (ANN) approaches, a sub-field of intelligent systems, are being widely used to solve a wide variety of problems in civil engineering applications. Topçu and Sarıdemir (2008c) were studied that prediction of compressive strength of concrete containing fly ash were investigate by using artificial neural networks and fuzzy logic. 180 concrete samples were prepared from 52 different mixes. These concrete mixtures contained Portland cement, fly ash and sand, crushed fine and coarse aggregate, water reducing and lime (CaO). High lime and low lime fly ashes were used by a ratio of 10, 20 and 40% in concrete mixture instead of Portland cement. In ANN and fuzzy logic models input data were curing periods (day), Portland cement, fly ash, sand, crushed fine and coarse aggregate, water reducing and lime. 7, 28 and 90 days concrete samples compressive strength was used as outputs in the models. The results showed that ANN and fuzzy logic methods could be used to predict concrete compressive strength. Kasperkiewicz et al. (1995) used fuzzy-ARTMAP type of ANNs in the prediction of high performance concrete strength properties. In the concrete mix, cement, super plasticizer, silica fume, water, fine and coarse aggregate were present. In the prediction the only purpose is to compute the 28 day compressive concrete strength. The results showed that neural network applications could be used instead of the conventional regression models. Lorenzi et al. (2003) were applied ANNs using back-propagation algorithm on some properties of concrete that were readily attained by ultrasonic tests. It is stated that predictions achieved from back-propagation ANN applications showed better results than the regression analysis, which is a conventional modelling technique. Most of ANNs applications in civil engineering focused on concrete properties such as workability of concrete, mechanical behavior and physical properties of concrete, effect of fly ash and silica fume on compressive strength (Lee, 2003; Bilim et al., 2009; Topçu and Sarıdemir, 2008a,b; Altun et al., 2008). It is well known that the physical and mechanical properties of cement affect concrete properties directly. But there are few studies in literature that ANN is used for estimating cement properties. It will be helpful to make further studies on the availability of ANNs in estimating cement properties, which is similar to the one made on estimating concrete properties. In this paper, ANN and regression technique were used in order to predict the compressive strength and flexural tensile strength of cement containing c class fly ash without performing any experiments. And the developed prediction model results and the experimental results were compared.

Regression technique

Regression technique (RT) is the modelling of the relationship between 1 or more measured variables and another variable which is genuinely considered to be related to the measured variable(s). In the regression technique, the influencing variable (that is, the variable that causes an apparent change in the other variable) is called as explanatory variable (or independent variable) and the variable which is influenced by the independent variable (that is, affected by the apparent change caused by the independent variable) is called dependent variable (Kalaycı, 2006). Regression models can be classified as linear and non linear models. However, non linear models can be transformed into linear models by various methods. To make a good prediction with the non linear regression models, you have to have preliminary information on the degree of the model or assume. The formulation of the equations of multiple linear regression is given in Equation 1.

$$Y = b_o + b_1X_1 + \ldots\ldots\ldots\ldots\ldots + b_nX_n + \varepsilon \quad (1)$$

In model equation,
Y = Dependent variable
X_i = Independent variable
b_i = Calculated coefficient parameters
ε = Error term

Artificial neural networks

ANN, imitating the functioning of human brain, is a tool of great importance in sample classification, pattern recognition and forecasting. ANN can learn via trial and error and so, to generalize.

A typical ANN model is a combination of layers made of neurons. Most widely used ANN type is multi layer perception. Multi layer perception (MLP) is composed of an input layer that takes the data in, an output layer that conveys the output of the network out and usually 1 but occasionally more than 1 hidden layers in between. In the input layer, input of the neurons are taken in from outside. Nevertheless, net input of a neuron in the hidden layers or the output layer is the sum of multiplications of all the input received (xi, I = 1, 2,...,n) by corresponding weights (wi, I = 1, 2,..,n), that is, $(\sum_i w_i.x_i)$; while output of a neuron is gotten after the net input is processed by the activation function (Lin and Lee, 1996; Zhang et al., 1998). A neuron is showed in Figure 1.

Numeric value for the output of neuron is calculated using Equation 2.

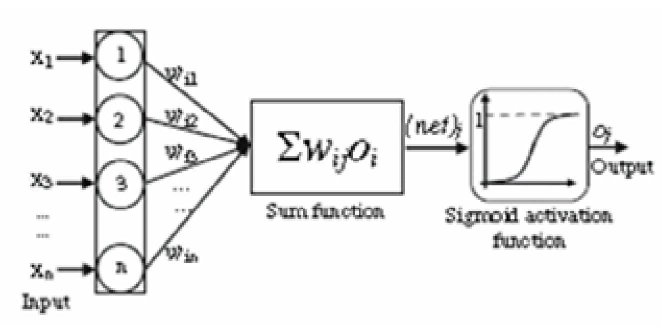

Figure 1. The artificial neuron model.

$$o = f(\sum_{i=1}^{n} w_i x_i + b) \quad (2)$$

Where n is the number of input nodes, f is the activation function, x_i is i^{th} (I = 1 ton) input variable, w_i's are weights for input nodes and b is weight of arc leading from the bias term whose values equal to 1 (Hamzaçebi and Kutay, 2005).

In order for an MLP to achieve a required task, network should be trained with data regarding the problem. Back propagation is a frequently used training algorithm. Important factors that affect the ANN performance can be listed as the number of input neurons, hidden neurons, output neurons and activation function. In a prediction problem based on cause and effect relationship, the number of input neurons is equal to the number of independent variables and the number of output neurons is equal to the number of dependent variables. To settle the number of hidden neurons heuristic approaches may be used or experimental design may be made. There are some proposed approaches in the literature to figure out the number of hidden neurons, which are not valid for the all problems. Let “n” be the number of input neurons, “m” be the number of output neurons and then one of the following approaches may be selected to settle the number of hidden neurons

i.) n (Tang and Fishwick, 1993)
ii.) 2n+1 (Lippman, 1987)
iii.) 2n (Wong, 1991)
iv.) $\sqrt{n*m}$ (Masters, 1993)
v.) $0{,}75*n$ (Baily and Thompson, 1990)

In the ANN designed for prediction problems, as a hidden layer activation function as a sigmoid or a hyperbolic tangent function is used. Furthermore, for the output layer activation function, generally, a linear function is used (Zhang et al., 1998).

Table 1. Chemical analysis results of fly ash.

Chemical composition	
SiO_2 (%)	47,77
Al_2O_3 (%)	11,95
Fe_2O_3 (%)	7,84
CaO (%)	12,95
MgO (%)	7,04
SO_3 (%)	2,59
Na_2O (%)	2,94
K_2O (%)	2,14

Table 2. Gradient and chemical composition of sand.

Chemical composition	%	Griddle pore size(mm)	Remaining
SiO_2	93.05	0.08	99.12
Al_2O_3	3.11	0.16	86.21
Fe_2O_3	0.37	0.5	65.74
CaO	0.17	1	33.02
MgO	0.03	1.6	5.23
SO_3	0.07	2	–
K_2O	1.5	Humidity	0.11
Na_2O	1.1		
LOI	0.57		

Experimental details

In this study CEM I 42.5 R cement and class C fly ash were used. The chemical analysis results of the fly ash used are given in Table 1.

CEN reference sand specified in TS EN 196-1 was used for the preparation of test samples and is silica sand whose gradient and chemical composition are presented in Table 2. The water amount used in the mixture for each group was determined through flow Table test in accordance with flow diameter specified in the standards of ASTM C230, ASTM C109 and ASTM C1437. The admixture proportions for the materials used in the preparation of samples are given in Table 3. Fly ash used in the study was put in the admixture replacing cement by the rates of 0, 5, 10, 15 and 20. Samples were first cured in a fog room at 20℃ for 24 h, and then demoulded and cured in water at 20 ± 2℃ until test time. Cement compressive and flexural tensile strength test was conducted on 2, 7 and 28th days and made on 4 samples with the size of 40 x 40 x 160 mm for each group. Compressive and flexural tensile strength tests were carried out in accordance with the rules specified in TS EN 196-1 standard. Compressive and flexural tensile strength measure-ments are made by using computer controlled compression machine and the loading speed for these measurements are chosen to be 1 kN/s and 50 N/s respectively. Compressive strength Rc and flexural tensile strength Rf were calculated by employing equation 3 and 4, respectively.

$$R_c = \frac{F_c}{1600} \quad (3)$$

Table 3. Mix proportions of cement sample.

Replaced fly ash	Water/Cement ratio	Sand (g)	Cement amount (g)	Water (ml)
%0	0.48	1350	450	216
%5	0.52	1350	450	234
%10	0.55	1350	450	247.5
%15	0.57	1350	450	256.5
%20	0.58	1350	450	261

Table 4. The input and output quantities used in the models.

Input variables	Data used In training and testing the models	
	Minimum	Maximum
Age of specimen (day)	2	28
Fly ash (%)	0	20
Unit weight (g/cm^3)	2.135	2.25
Compressive strength (MPa)	22.23	51.285
Tensile strength (MPa)	3.809	7.409

Where;
Rc =Compressive strength (MPa),
Fc = Maximum breaking load (N),
1600 = Sample area (mm²)

$$R_f = \frac{1,5.F_f.l}{b^3} \quad (4)$$

Where;
Rf = Flexural tensile strength, (MPa)
b = Edge length of prism square section (mm),
F_f = Force applied when prism broken (N),
l = Distance between support rollers (mm)

APPLICATION AND RESULTS

Prediction with RT

The Linear regression model is used in the prediction of compressive and flexural tensile strength. The reason non-linear regression models are not preferred here is that there is no information about the data structure. Not knowing the degree of the non-linear regression model previously necessitated the use of linear regression models. In the formulated model, the independent variables are age of specimen, fly ash and unit weight of mortars and the dependent variable is the compressive and flexural tensile strength. 51 data were used in forming regression model and 9 data were used in testing model equation obtained. The limit values of variables used in the multiple linear regression models are listed in Table 4. The predicted compressive and flexural tensile strength values are represented by Rc and Rf respectively. The prediction model used in this study is shown in equation 5. Where X_1 is age of specimen, X_2 is the fly ash and X_3 is the unit weight of the samples. The equations with the coefficients obtained from multiple linear regression analysis are given in Table 5.

$$Rc, Rf = b_1X_1 + b_2X_2 + b_3X_3 \quad (5)$$

All results obtained from experimental studies and predicted by using the training and testing results of the RT, for compressive and flexural tensile strength were given in Figures 2 and 3. The linear least square fit line, its equation and the regression coefficient (R^2) values were shown in these Figures for the training and testing data. The statistical values of root mean square error (RMSE), R^2 and mean absolute % error (MAPE) including all the station for both training and testing for RT are given in Table 6.

As shown in Figures 2 and 3, moderate results were obtained from the RT model. The statistical parameter values of RMSE, R^2 and MAPE showed obviously this situation (Table 6). While the statistical values of RMSE, R^2 and MAPE from training in the RT model were found as 2.836121, 0,908 and 0.176883, respectively, these values were found in testing as 3.416964, 0.8604 and 0.759968, respectively for compressive strength values. For flexural tensile strength values, the statistical values of RMSE, R^2 and MAPE from training in the model were found as 0.462994, 0.740 and 0.188729, respectively, these values were found in testing as 0.584094, 0.5989 and 0.873357, respectively. R^2 values were seen to decrease in test setting considerably and the obtained RT models fell behind estimating the values of compressive and flexural tensile strength.

Prediction with ANN

ANN model developed in this research has three neurons in the input layer and 2 neurons in the output layer as illustrated in Figure 4. Two hidden layer with for first layer 5 neurons and second layer 4 neurons were used in the architecture because of its minimum % error values for training and testing sets. While modeling networks, fly ash content (%), age of specimen (days), and unit weight (g/cm^3) were used as input parameters and tensile and the compressive strengths (N/mm²) were used as output parameters.

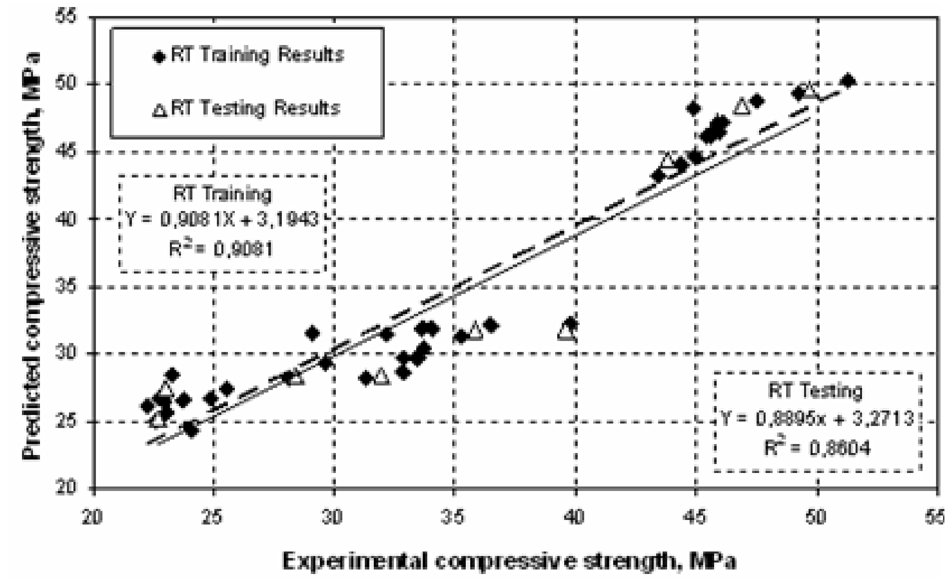

Figure 2. Comparison of Rc experimental results with training and testing results of RT.

Table 5. The equations of multiple linear regression models.

Experiment	Regression Coefficients R^2	Model equations $Y = a+bX_1+cX_2+dX_3$
Compressive strength	0,908	$Rc = -81,827+0,739X_1-0,192X_2+49,69X_3$
Flexural tensile strength	0,740	$Rf = -25,432+0,061X_1-0,019X_2+13,767X_3$

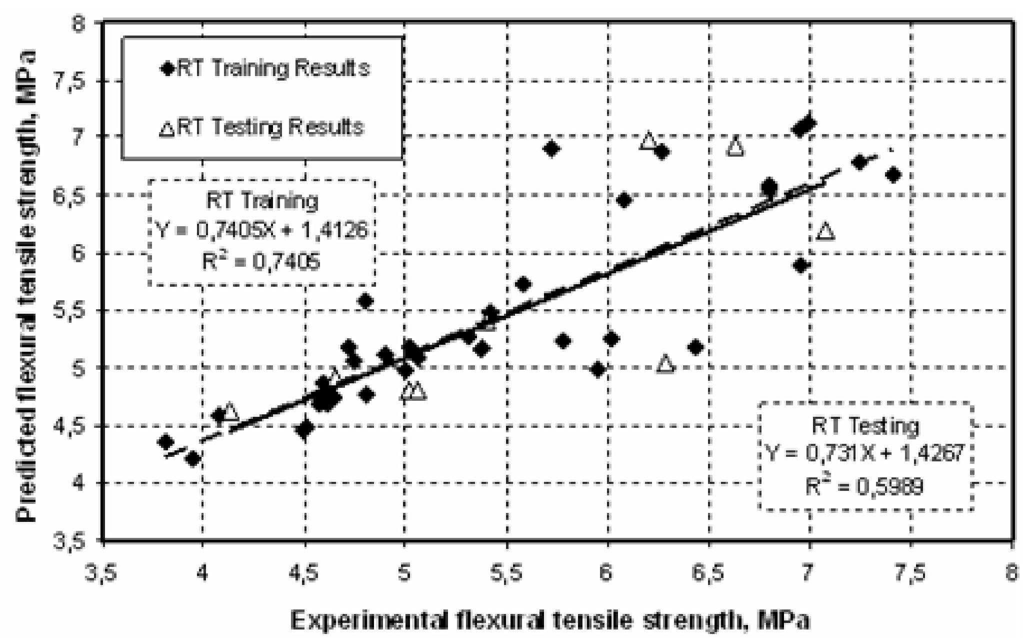

Figure 3. Comparison of Rf experimental results with training and testing results of RT.

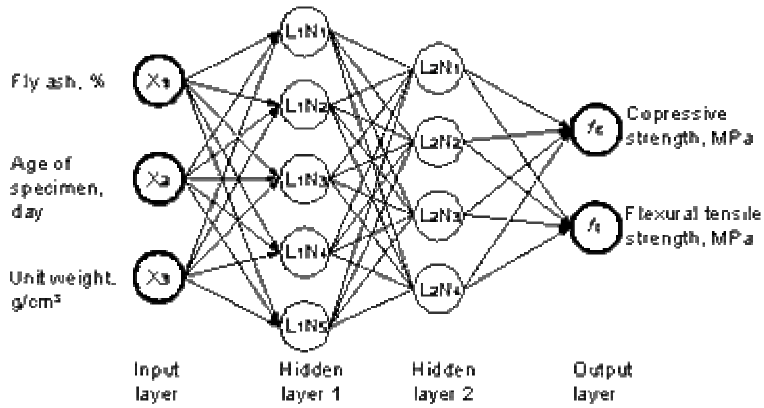

Figure 4. Structure of the network for prediction of compressive strength.

Table 6. The statistical values of proposed RT model.

Statistical parameters	Training set		Testing set	
	Compressive strength	Flexural tensile strength	Compressive strength	Flexural tensile strength
RMSE	2,836121	0,462994	3,416964	0,584094
R^2	0,908	0,740	0,8604	0,5989
MAPE	0,176883	0,188729	0,759968	0,873357

Table 7. The values of parameters used in the multilayer neural network model.

Parameters	ANN
Number of input layer neurons	3
Number of hidden layer	2
Number of hidden layer 1 neurons	5
Number of hidden layer 2 neurons	4
Number of output layer neuron	2
Momentum rate	0,1
Learning rate	0,001
Error after learning	0,000105599
Learning cycle	5000

For training set 51 samples were selected and the residual data (9 samples) were selected as testing set. The limit values of input and output variables used in the multilayer feed-forward neural network model are listed in Table 4. The values of the training and test data were normalized between 0 and 1 using equation 6.

$$F = (F_i - F_{min}) / (F_{max} - F_{min}) \quad (6)$$

In this equation F represents normalized value, F_i represents i value of measured values and F_{max} and F_{min} used in feed-forward with 2 hidden layers. Logarithmic sigmoid transfer function was used as the activation function for hidden layers and output layers.

Learning rate and momentum rate values were determined and the model was trained through iterations. The values of parameters obtained in the multilayer feed-forward neural network model are given in Table 7. The trained model was only tested with the input values and the results found were close to experiment results.

All results obtained from experimental studies and predicted by using the training and testing results of the ANN, for compressive and flexural tensile strength were given in Figures 5 and 6. The linear least square fit line, its equation and the R^2 values were shown in these Figures for the training and testing data. The statistical values of RMSE, R^2 and MAPE including all the station for both training and testing for RT are given in Table 8.

As seen in Figures 6 and 7, good results were obtained from the multilayer feed-forward neural network model. The statistical parameter values of RMSE, R^2 and MAPE showed obviously this situation (Table 8). While the statistical values of RMSE, R^2 and MAPE from training in the multilayer feed-forward neural network model were found as 0.380001, 0.9983 and 0.022757, respectively, these values were found in testing as 1.936772, 0.9557 and 0.411987, respectively for compressive strength values. For Flexural tensile strength values, the statistical values of RMSE, R^2 and MAPE from training in the ANN model was found as 0.094306, 0.9912 and 0.024368, respectively,

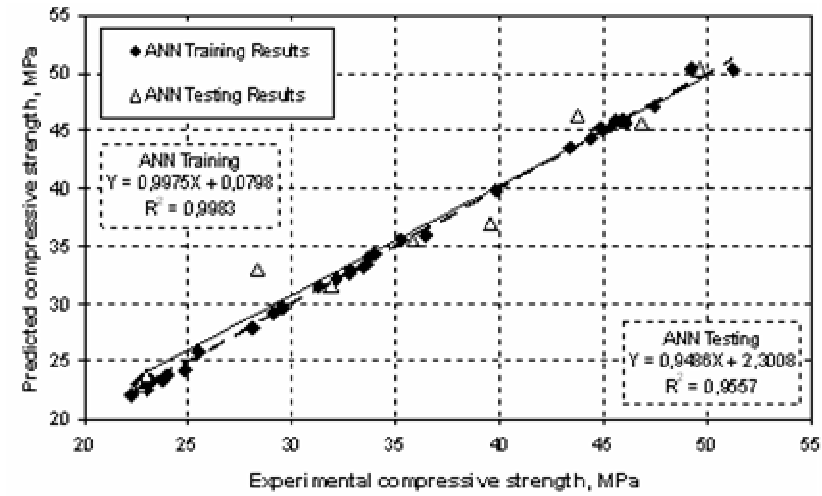

Figure 5. Comparison of *Rc* experimental results with training and testing results of ANN.

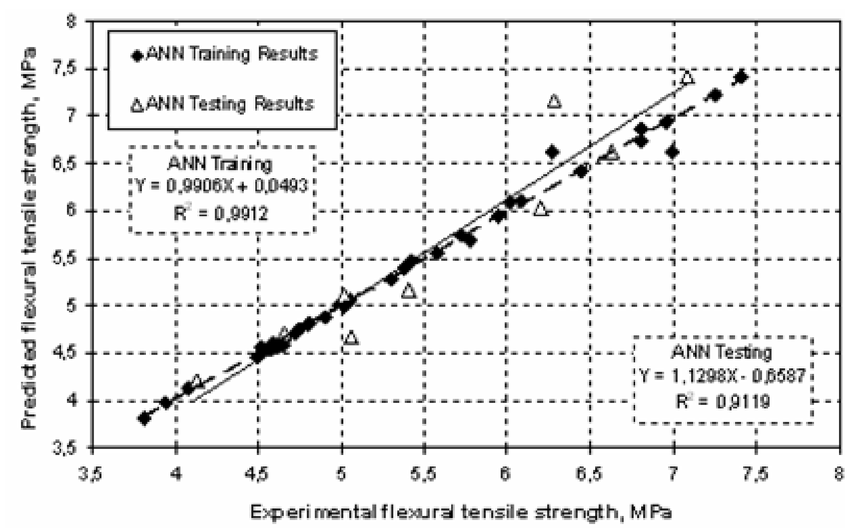

Figure 6. Comparison of *Rf* experimental results with training and testing results of ANN.

these values were found in testing as 0.336909, 0.9119 and 0.4143728, respectively.

All of the statistical values in Table 9 show that the proposed the multilayer feed-forward neural network model are suitable and predict the compressive and flexural tensile strength values very close to the experimental values. This finding is verified in other studies of literature. Topçu and Sarıdemir (2008c) were studied that prediction of compressive strength of concrete containing fly ash were investigate by using artificial neural networks and fuzzy logic. The results showed that ANN and fuzzy logic methods could be used to predict concrete compressive strength. Kasperkiewicz et al. (1995) used fuzzy-ARTMAP type of ANNs in the prediction of high performance concrete strength properties. The results showed that neural network applications could be used instead of the conventional regression models. Lorenzi et al. (2003) were applied ANNs using back-propagation algorithm on some properties of concrete that were readily attained by ultrasonic tests. It is stated that predicttions achieved from back-propagation ANN applications showed better results than the RT.

Comparison prediction techniques

The experimental compressive and flexural tensile

Table 8. The statistical values of proposed ANN model.

Statistical parameters	Training set		Testing set	
	Compressive strength	Flexural tensile strength	Compressive strength	Flexural tensile strength
RMSE	0.380001	0.094306	1.936772	0.336909
R^2	0.9983	0.9912	0.9557	0.9119
MAPE	0.022757	0.024368	0.411987	0.443728

Table 9. Testing data sets for comparison of experimental results with testing results predicted from models.

Input			Output					
Age of specimen (day)	Fly ash (%)	Unit weight (g/cm^3)	Compressive strength (MPa)			Flexural tensile strength (MPa)		
			Experiment data	RT	ANN	Experiment data	RT	ANN
2	0	2.188	28.35	29.02	32.99	5.01	4.88	5.11
2	10	2.209	23.00	26.96	23.76	4.65	3.88	4.71
2	20	2.202	22.64	24.93	22.81	4.13	2.88	4.21
7	0	2.183	39.56	32.87	37.00	6.28	5.22	7.16
7	10	2.222	35.79	30.79	35.46	5.40	4.23	5.16
7	20	2.193	31.90	28.78	31.57	5.06	3.22	4.68
28	0	2.227	49.67	48.95	50.25	6.63	6.68	6.62
28	10	2.243	46.89	46.89	45.56	6.20	5.68	6.03
28	20	2.200	43.79	44.90	46.33	7.08	4.67	7.41

Table 10. The prediction performances of both techniques for the testing set.

Prediction models	Compressive strength (MPa)			Flexural tensile strength(MPa)		
	MAPE	R^2	RMSE	MAPE	R^2	RMSE
RT	0.759968	0.8604	3.416964	0.873357	0.5989	0.584094
ANN	0.411987	0.9557	1.936772	0.443728	0.9119	0.336909

strength values in the test sample and the predicted strength values by both techniques are shown in Table 8. In addition, the performance parameters of RT and ANN techniques are given in Table 10. As can be seen from Table 9, the smallest prediction errors are observed in ANN technique according to the performance criteria such as MAPE, R^2 and RMSE. The prediction success of ANN technique is much better than the regression technique.

The best value of R^2 is 0.9557 for testing set in the ANN model. The minimum value of R^2 is 0.5989 for testing set in the RT model. All of the statistical values in Table 10 show that the proposed the multilayer feed-forward neural network model is suitable and predict compressive and flexural tensile strength values very close to the experimental values than RT.

Conclusion

In his study, artificial neural networks and regression techniques were used for the prediction the compressive and flexural tensile strength values of mortars containing various amount class C fly ashes. In the model developped in artificial neural networks system, a multilayered feed-forward neural network with a back-propagation algorithm was used. In the multilayer feed-forward neural network model, 2 hidden layers were selected. In the first hidden layer 5 neurons and in the second hidden layer 4 neurons were determined. Furthermore, in the model developed in regression technique, multiple linear regression was used. These models were trained with input and output data. Using only the input data in trained models the compressive and flexural tensile strength values of mortars containing fly ash were found. The compressive and flexural tensile strength values predicted from testing, for the multilayer feed-forward neural network are very close to the experimental results than predicted values of regression model. The statistical parameter values of RMSE, R^2 and MAPE have shown obviously this situation.

As a result, compressive and flexural tensile strength values of mortars containing various amount class C fly ash can be predicted in a quite short period of time with tiny error rates by using the multilayer feed-forward neural network models than regression techniques. The conclusions have demonstrated that artificial neural networks are practicable methods for predicting compressive and flexural tensile strength values of mortars containing class C fly ash.

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