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Analyzing the compressive strength of clinker mortars using approximate reasoning approaches – ANN vs MLR

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Abstract. In this paper, Artificial Neural Networks (ANN) and Multiple Linear Regression (MLR) models were discussed to determine the compressive strength of clinker mortars cured for 1, 2, 7 and 28 days. In the experimental stage, 1288 mortar samples were produced from 322 different clinker specimens and compressive strength tests were performed on these samples. Chemical properties of the clinker samples were also determined. In the modeling stage, these experimental results were used to construct the models. In the models tricalcium silicate (C_3S), dicalcium silicate (C_2S), tricalcium aluminate (C_3A), tetracalcium alumina ferrite (C_4AF), blaine values, specific gravity and age of samples were used as inputs and the compressive strength of clinker samples was used as output. The approximate reasoning ability of the models compared using some statistical parameters. As a result, ANN has shown satisfying relation with experimental results and suggests an alternative approach to evaluate compressive strength estimation of clinker mortars using related inputs. Furthermore MLR model showed a poor ability to predict.

Keywords: clinker; prediction; compressive strength; artificial neural networks; multi linear regression

1. Introduction

Concrete is one of the most widely used construction material, owing to its good durability to cost ratio. The most important parameter on concrete performance is the properties of cement used in concrete production. Cement is the most produced and used binding material in the world with its 1.6 billion tons of annual production (Bilim 2011; Karakurt & Topçu 2011). Cement production has undergone a tremendous development from its beginnings some 2000 years ago. While the use of cement in concrete has a very long history, the industrial production of cements started in the middle of the 19th century, first with shaft kilns, which were later on replaced by rotary kilns as standard equipment worldwide (Schneider Romer *et al*. 2011). Portland cement is a binding material produced by grinding clinker with gypsum. Anhydrous Portland cement is essentially made of a synthetic rock, referred to as clinker, which contains at least four major phases. These

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phases are tricalcium silicate (C_3S), dicalcium silicate (C_2S), tricalcium aluminate (C_3A) and tetracalcium alumina ferrite (C_4AF) (Neville 1981; Dunstetter de Noirfontaine *et al*. 2006).

Mineralogical and microstructure properties are mostly examined on coarse clinker particles and obtained results such as amount and dimension of mineral phases, porosity and some operational parameters of clinker manufacturing are usually dealt with clinker grind ability. Clinker or cement microstructure data could also help to predict cement service properties, particularly strength. But the combined effect of these micro structural parameters on strength should be considered otherwise the correlation may be low if these parameters are evaluated in isolation against compressive strength. It is apparent that several factors may play different roles together on service properties (Celik Oner *et al*. 2007).

Designers utilize principles of science and mathematics to develop specific technologies. These technologies are then used to create engineered tools such as products, structures, machines, processes or entire systems. It has already been seen that different tasks in engineering problem solving require different analysis (Krishnamoorthy & Rajeev 1996).

Nowadays, artificial intelligence methods are much popular in engineering sciences. One of the most popular artificial intelligence methods is ANN. ANN is a computational modeling method that tries to simulate the structure or functional aspects of biological neural networks. ANN can exhibit amazing capability in modeling the human brain. Generally, ANN model consists of a number of interconnected group of artificial neurons, each of which is fully connected to the other through connection weights. These weights, present the effect of an input parameter in the previous layer on the process element, can be adjusted to produce an output needed. ANN which is sometimes called as black-box modeling approach is an adaptive system that can be change its model according to relevant information that flows through the network during the learning phase. ANN can be used to model nearly any complex relationships between inputs and outputs in data (Duan Kou *et al*. 2013).

Recently, artificial neural networks has been extensively using in the fields of civil engineering applications especially cement and concrete properties estimation (Topçu & Sarıdemir 2008; Molero Segura *et al*. 2009; Özcan Atiş *et al*. 2009; Sarıdemir 2009; Sarıdemir Topçu *et al*. 2009; Başyigit Akkurt *et al*. 2010; Erdem 2010; Önal & Öztürk 2010; Slonski 2010; Gencel Kocabas *et al*. 2011; Kyriazopoulos Anastasiadis *et al*. 2011; Nazari & Riahi 2011; Siddique Aggarwal *et al*. 2011; Alexandridis Triantis *et al*. 2012; Amani & Moeini 2012; Khan 2012; Madandoust Bungey *et al*. 2012; Öztürk & Turan 2012; Shah Alsayed *et al*. 2012; Triantis Stavrakas *et al*. 2012; Uysal & Tanyildizi 2012; Bal & Buyle-Bodin 2013; Boğa Öztürk *et al*. 2013; Duan Kou *et al*. 2013; Mashrei Seracino *et al*. 2013).

Alexandridis Triantis *et al*. (2012), presented a non-destructive method to predict the compressive strength of cement-based materials by studying the appearance of weak electrical signals (Kyriazopoulos Anastasiadis *et al*. 2011; Triantis Stavrakas *et al*. 2012) at specimens that are under mechanical stress. The result of their study showed that the ultimate compressive strength can be successfully predicted using ANN without destructive tests. The result of their study showed that the ultimate compressive strength can be successfully predicted using ANN without destructive tests. Önal O and Öztürk AU studied an artificial neural network analysis to establish a relationship between microstructural characteristics and compressive strength values of cement mortar. The developed model showed that a strong correlation between the microstructural properties of cement mortar and compressive strengths can be established by using ANN as non-linear statistical data modeling tool (Önal & Öztürk 2010). Sarıdemir developed two models (ANN and Fuzzy logic) to predict the compressive strength of mortars containing metakaolin at the age of 3, 7, 28, 60 and 90 days. He used the data gathered from literature (179 specimens produced with 46 different mixture proportions). The results in the multilayer feed-forward neural networks developed in his research showed that neural networks system has strong potential for predicting compressive strength of mortars (Sarıdemir 2009). Nazari *et al* studied the multilayer feed forward neural networks and genetic programming to predict split tensile strength and percentage of water absorption of concretes containing TiO_2 nanoparticles. Result showed that neural network predicted better results (Nazari and Riahi 2011). Khan studied the applicability of artificial neural network for the prediction of compressive strength, tensile strength, gas permeability and chloride ion penetration of high performance composite cementitious systems. Results showed that results of developed model and experimental have a good correlation between each other (Khan 2012). Dantas *et al* developed an Artificial Neural Networks (ANNs) model for predicting the compressive strength, at the age of 3, 7, 28 and 91 days, of concretes containing Construction and Demolition Waste (CDW). They used a total of 1178 data to construct the models. The training and testing phases of their study strongly show the potential use of ANN to predict 3, 7, 28 and 91 days compressive strength of concretes containing CDW (Dantas Batista Leite *et al*. 2013).

In this presented paper, Artificial Neural Network (ANN) and Multiple Linear Regression (MLR) models were discussed to determine the compressive strength of clinker mortars. For constructing this models, 322 different mixtures with 1288 specimens of the 1, 2, 7 and 28 days compressive strength test results of clinker mortars, were used in training and testing. In training and testing of the models the input of C_3S, C_2S, C_3A, C_4AF, Blaine, specific gravity and age of samples were entered into the system while the output of compressive strength values were entered on the other hand. The model was trained with 201 experimental data results. Latterly, the remainders were used as only experimental input values for testing.

2. Experimental study

2.1. Specimens

The clinkers were produced in the Bursa Cement Factory (Turkey) and all experiments and analysis were performed in the factory. Chemical and physical analyses were conducted on samples used in the experiments. Chemical analyses of clinkers were performed on ARL 9900 X-ray workstation (XRF+XRD). Surface areas were determined as Blaine values by Toni Technik 6565 and specific gravity were determined by Quantachrome MVP-3. The results obtained from the chemical analyses of 322 different clinkers were given in Table 1.

Table 1 Chemical composition of clinkers

Chemical composition: wt.%	Minimum	Maximum	Chemical composition: wt.%	Minimum	Maximum
SiO_2	18.67	21.58	Na_2O	0.19	0.53
Al_2O_3	6.12	6.82	K_2O	0.01	0.75
Fe_2O_3	3.29	3.96	Cl^-	0.005	0.06
CaO	64.85	68.06	Loss on ignition	0.23	0.45
MgO	0.77	1.54	Reactive CaO	0.36	3.22

SO_3	0.24	1.05

Table 2 The input and output parameters and quantities used in models.

Input parameters	Data used in training and testing the models	
	Minimum	Maximum
C_3S (%)	52.32	67.25
C_2S (%)	6.29	21.80
C_3A (%)	10.35	11.73
C_4AF (%)	10.01	12.05
Blaine (cm^2/g)	2810	3250
Specific gravity	3.12	3.27
Period of curing (Days)	1	28
Output value (MPa)	4	62.20

In the preparation of clinker mortar mixtures for compressive strength experiments, 450 g of clinker, 1350 g of standard sand and 225 ml of water were used in each mortar mixture according to TS EN 196-1. Prepared clinker mortars were poured into three-segmented 40x40x160 mm sized rectangular prism molds. Prepared samples were waited in the laboratory for 24 hours. At the end of 24-hour period, the samples were taken out of the molds and placed in water pools to get cured and prepared for the compressive strength experiments. Compressive strengths of each clinker mortars were measured at the end of 1, 2, 7 and 28 days using Atom Technic device. The minimum and maximum values of the experimental results used in modeling are given in Table 2.

4. Regression Technique

Regression technique 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 nonlinear models. However, nonlinear models can be transformed into linear models by various methods. To make a good prediction with the nonlinear regression models, you have to have preliminary information on the degree of the model or assume. The multiple linear regression model is an extension of a simple linear regression model to incorporate two or more explanatory variable in a prediction equation for a response variable. Multiple regression modeling is now a mainstay of statistical analysis in most fields because of it's power and flexibility (Brant 2007).

The formulation of the equations of multiple linear regression is given in Equation 1 (Subaşı 2009).

$$Y = b_0 + b_1X_1 + \cdots \ldots\ldots + b_nX_n + \varepsilon \quad (1)$$

In model equation,
Y = Dependent variable

Xi = Independent variable
bi = Calculated coefficient parameters
ε = Error term

5. Comparison criteria for the model

In the present study, the adequacy of the developed ANN model was evaluated by considering three statistical evaluation criteria. These statistical parameters are coefficient of determination (R^2) Eq. 2, Root Mean Squared Error (RMSE) Eq. 3 and Mean Absolute Errors (MAE) Eq. 4. Besides, the matching figures were drawn for both training and testing data to see relationship between model and experimental results.

$$R^2 = 1 - \{[\sum_{i=1}^{n}(Y_{i(m)} - Y_{i(p)})^2]/[\sum_{i=1}^{n}(Y_{i(m)} - Y_{i(mean)})^2]\} \tag{2}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Y_{i(m)} - Y_{i(p)})^2} \tag{3}$$

$$MAE = \frac{1}{N}\sum_{i=1}^{N} | Y_{i(m)} - Y_{i(p)} | \tag{4}$$

Here *m* is the measured values, *p* is the predicted values, *mean* is the average measured values and *N* is the number of data. The statistical values of R^2, RMSE and MAE for all the data sets are given related figures.

6. Developed ANN model structure, parameters and results

The ANN modeling consists of two steps: first step is to train the network; second step is to test the network with data, which were not used in training step. Neural networks have been trained to perform complex functions in various fields of application including pattern recognition, identification, classification, speech, vision and control systems (Terzi 2007)

ANN model developed in this research has seven neurons (variables) in the input layer and one neuron in the output layer as illustrated in Fig. 3. Some of the architectures with different number of neurons studied here in hidden layer/layers and their correlations with experimental results were investigated. The results of the comparison of the most successful ANN architectures tested in this study are given in Table 3. As seen in Table 3. minimum percentage error values were found through two hidden layer with 10 neurons of first layer and 5 neurons of second layer both training and testing sets.

While modeling networks, C_3S, C_2S, C_3A, C_4AF, blaine values, specific gravity and age of samples were used as inputs and the compressive strength of clinker samples was used as output. While modeling, 1087 samples were selected as training set and 201 data were selected as test set.

The values of the training and test data were normalized between 0 and 1 using equation 5.

Table 3 Comparison results of the most successful ANN models tested in this study

ANN architectures	7-8-6-1	7-9-5-1	7-9-6-1	7-10-3-1	7-10-5-1	7-10-5-1
R^2 (training)	0.78	0.84	0.85	0.92	0.98	0.94
R^2 (testing)	0.75	0.81	0.83	0.87	0.98	0.91

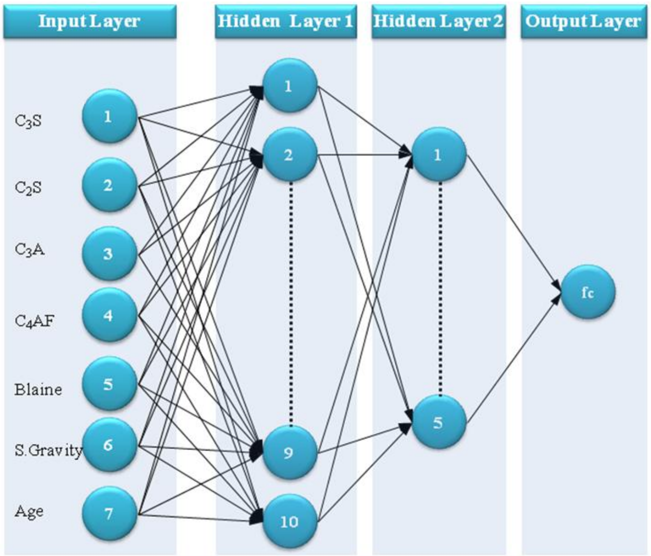

Fig. 3 ANN model developed in this research

While modeling networks, C_3S, C_2S, C_3A, C_4AF, blaine values, specific gravity and age of samples were used as inputs and the compressive strength of clinker samples was used as output. While modeling, 1087 samples were selected as training set and 201 data were selected as test set. The values of the training and test data were normalized between 0 and 1 using equation 5.

$$F = (F_i - F_{\min})/(F_{\max} - F_{\min}) \quad (5)$$

In this equation F represents normalized value, F_i represents *i.* value of measured values and F_{max} and F_{min} represent maximum and minimum values of measured values.

Feedforward artificial neural networks (ANNs) are currently being used in a variety of applications with great success. The first main advantage of feedforward artificial neural networks is that they do not require a user-specified problem solving algorithm but instead they “learn” from examples, much like human beings. The second main advantage of feedforward artificial neural networks is that they possess an inherent generalization ability (Benardos & Vosniakos 2007).

In this study, the back-propagation learning algorithm was used in feed-forward with two hidden layer. Logarithmic sigmoid transfer function was used as the activation function for hidden layers and output layer. The learning rate and momentum are the parameters that affect the speed of convergence of the back-propagation algorithm. A learning rate of 0.001 and momentum 0.1 were fixed for selected network. The details of modeling parameters are given in Table 4.

Table 4 The values of parameters used in model

Parameters	Values
Number of input layer neurons	7
Number of hidden layer	2
Number of first hidden layer neurons	10
Number of second hidden layer neurons	5
Number of output layer neuron	1

Table 5 The R^2, MAE, RMSE statistics of comparison (ANN model and experimental results)

	Statistical parameters		
	R^2	MAE	RMSE
Training stage	0.98	1.50	1.93
Testing stage	0.98	1.74	2.26

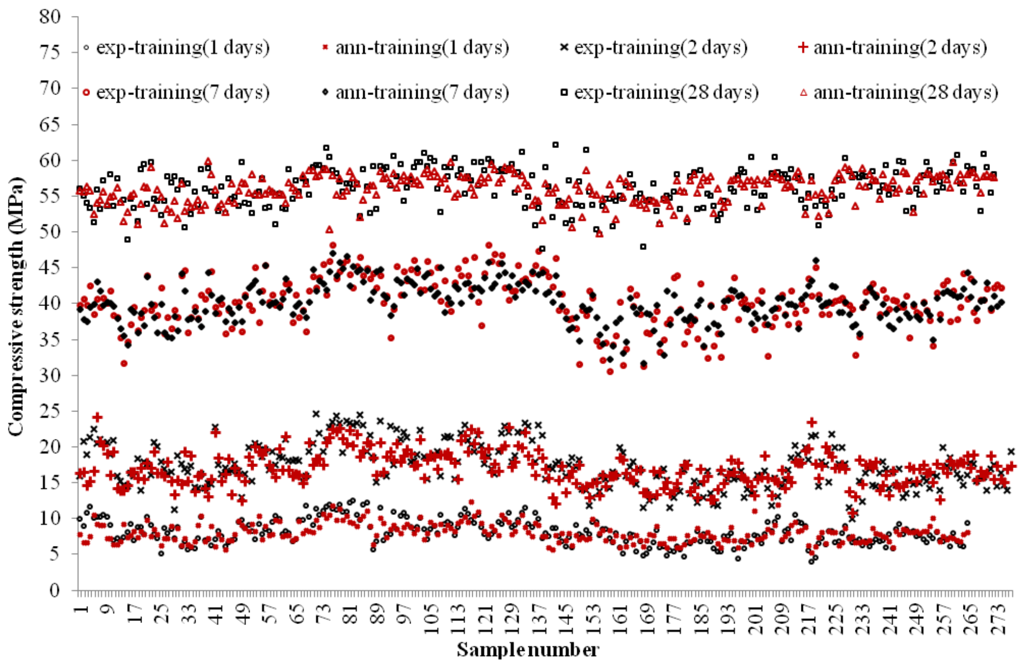

Fig. 4 Matching of results for training set (ANN training)

The trained networks were used to run a set of test data. The ANN (7-10-5-1) has the best correlation with experimental results both training and testing sets. The representation of the network is as follow: in the model of 7-10-5-1, first number 7 represents the number of neurons in input layer, the number 10 represents the number of neurons in the first hidden layer, the number 5 represents the number of neurons in the second hidden layer and the last number 1 represents the number of neuron in output layer. Matching figure, correlation figure for training set and correlation figure for testing set are displayed in Figure 4-5-and 6, respectively. The R^2, MAE and RMSE statistics obtained by comparing ANN model and experimental results by using Eq. 2,3 and

4 are presented in Table 5.

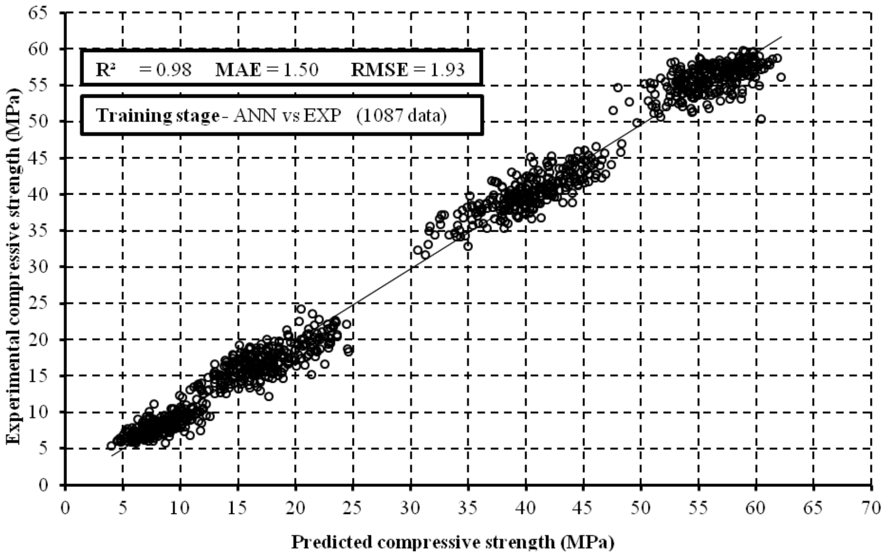

Fig. 5 Relationship between measured and predicted compressive strengths (ANN training)

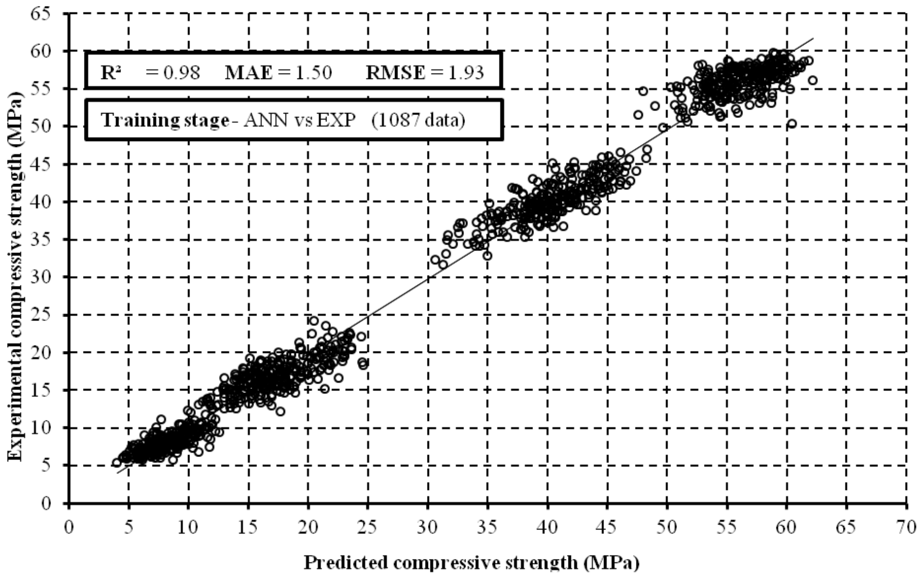

Fig. 6 Relationship between measured and predicted compressive strengths (ANN testing)

7. Statistical analysis and results

Tricalcium silicate, dicalcium silicate, tricalcium aluminate, tetracalcium alumina ferrite, blaine values, specific gravity and age of samples were selected as independent and the compressive strengths of clinker samples were selected as dependent variables to determine regression

Table 6 MLR model summary

Model	R	R^2	Adjusted R^2	Std. Error of the Estimate
1	0.894	0.800	0.792	8.81418

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients
		B	Std. Error	Beta
1	(Constant)	35.968	119.930	
	C_3S	1.138	0.915	0.182
	C_2S	0.588	0.900	0.092
	C_3A	-2.935	2.856	-0.036
	C_4AF	4.351	1.974	0.082
	Blain	-0.005	0.008	-0.021
	Specific Gravity	-30.622	25.066	-0.043
	Age	1.555	0.057	0.883

a. Predictors: (Constant), Age, Blaine, C_2S, Specific Gravity (SG), C_3A, C_4AF, C_3S

b. Dependent Variable: Compressive Strength

$$CS=35.968+1.138*C_3S+0.588*C_2S-2.935*C_3A+4.351*C_4AF-0.005*BL.-30.622*SG.+1.555*A \quad (6)$$

Table 7 The R^2, MAE, RMSE statistics of comparison (MLR analysis and experimental results)

	Statistical parameters		
	R^2	MAE	RMSE
Training stage	0.77	7.21	8.96
Testing stage	0.79	7.12	8.64

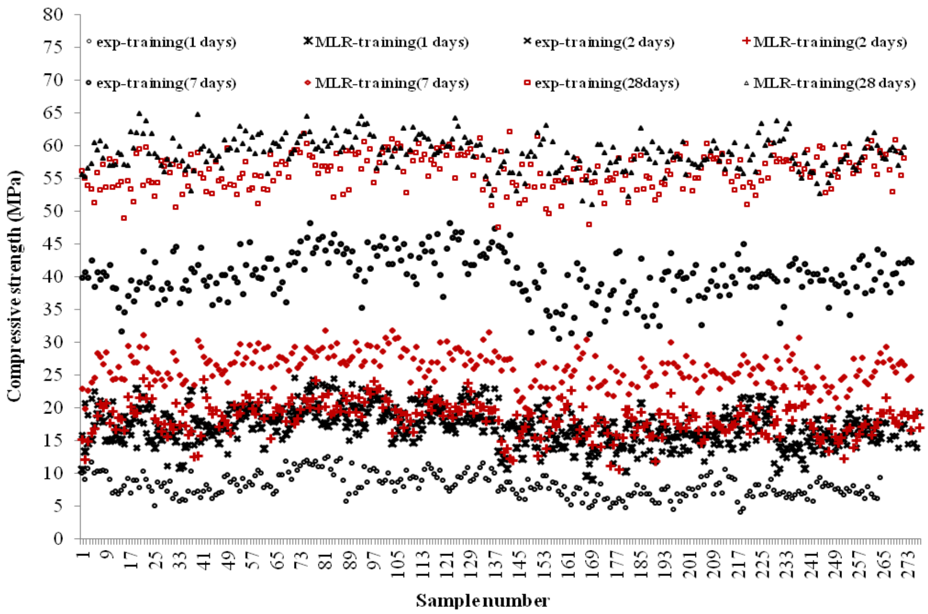

Fig. 7 Matching of results for training set (MLR training)

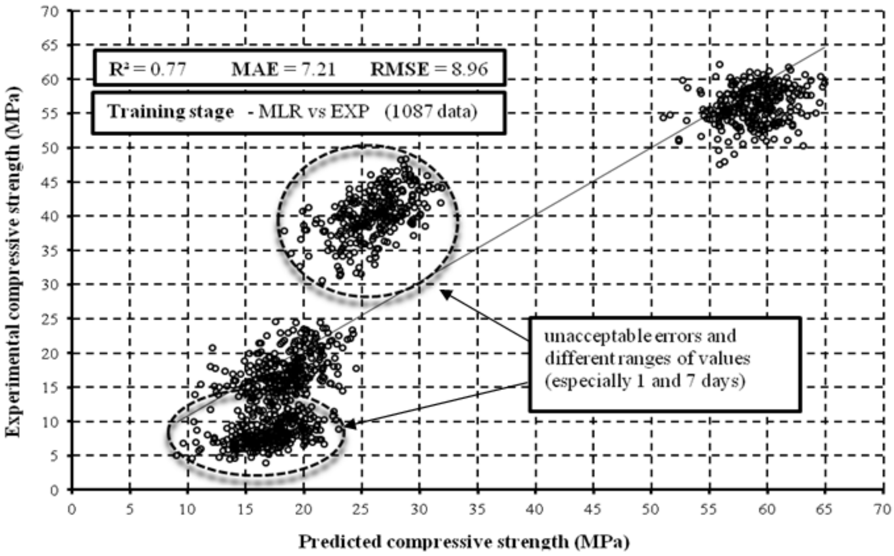

Fig. 8 Relationship between measured and predicted compressive strengths (MLR training)

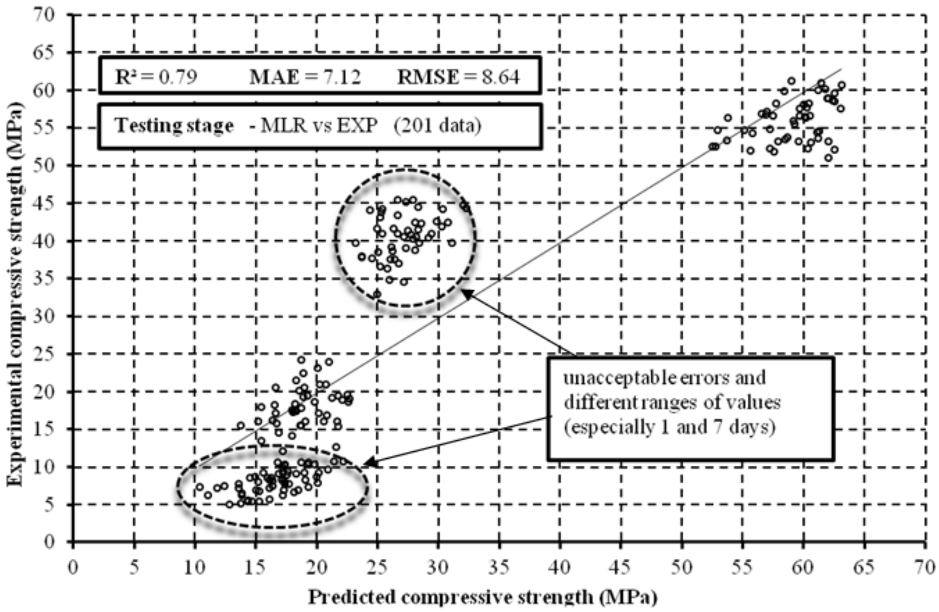

Fig. 9 Relationship between measured and predicted compressive strengths (MLR testing)

equation. A multiple linear regression (MLR) analysis was performed and an empirical correlation was developed to predict compressive strength of clinker mortars. In the model 1087 of 1288 experimental data selected for training the MLR analysis and 201 experimental data used for comparison of the experimental and statistical results. The resulting correlation at training stage is given in Eq. 6 and the regression model summary is listed in Table 6.

Where; CS is compressive strength (MPa), C_3S is tricalcium silicate, C_2S is dicalcium silicate, C_3A is tricalcium aluminate, C_4AF is tetracalcium alumina ferrite, BL is blaine values, SG is specific gravity and A is age of samples. Experimental compressive strength values were compared with the predicted values obtained from Eq. 1. (Figs. 7-8-9). The R^2, MAE and RMSE statistics obtained by comparing MLR analysis and experimental results by using Eq. 2,3 and 4 are presented in Table 7.

8. Conclusions

The potential of the Artificial Neural Network (ANN) and well known statistical method Multiple Linear Regression (MLR) technique were discussed for estimation the compressive strength of clinker mortars cured for 1, 2, 7 and 28 days. While developing the models 1087 experimental data (randomly selected) were used for training and 201 experimental data (the residual data) were used for testing. When comparing the prediction results and the experimental results in the training stage of ANN model, R^2, RMSE and MAE were found as 0.98, 1.93 and 1.50 respectively. In addition, these values were found as 0.77, 8.96 and 7.21 for comparing the MLR and experimental results in the training stage. Similarly comparisons were done at the test stage and R^2, RMSE and MAE were found as 0.98, 2.26 and 1.74 for ANN-Exp. comparison and 0.79, 8.64 and 7.12 for MLR-exp comparison respectively. Also, many unacceptable errors were seen when the matching figure evaluated for MLR-exp comparison especially 1 and 7 days results. According to the results, it can be concluded that MLR is not appropriate to use for this kind of application. When the results evaluated for ANN model, the results obtained from ANN model were very close to the experimental results.

As a result, this study shows that ANN can be used as a practical method for predicting the compressive strength values of clinker mortars cured for 1, 2, 7 and 28 days by using C_3S, C_2S, C_3A, C_4AF, blaine values, specific gravity and age of samples as inputs.

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