

## MLR & ANN approaches for prediction of compressive strength of alkali activated EAFS

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**Abstract.** In this study alkali activation of Electric Arc Furnace Slag (EAFS) is studied with a comprehensive test program. Three different silicate moduli (1-1.5-2), three different sodium concentrations (4%-6%-8%) for each silicate module, two different curing conditions (45%-98% relative humidity) for each sodium concentration, two different curing temperatures (400°C-800°C) for each relative humidity condition and two different curing time (6h-12h) for each curing temperature variables are selected and their effects on compressive strength was evaluated then regression equations using multiple linear regressions methods are fitted. And then to select the best regression models confirm with using the variables, the regression models compared between itself. An Artificial Neural Network (ANN) models that use silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables, are formed. After the investigation of these ANN models' results, ANN and multiple linear regressions based models are compared with each other. After that, an explicit formula is developed with values of the ANN model. As a result of this study, the fluctuations of data set of the compressive strength were very well reflected using both of the methods, multiple linear regression with quadratic terms and ANN.

**Keywords:** alkali activation; electrical arc furnace slag; regression; ANN

### 1. Introduction

Cement based materials are among the most important materials in construction industry. With increasing usage of cement based materials, production of cement also has been increased. So that consideration of environmental impacts and sustainable developments have been paid great attention by scientists (Rostami and Behfarnia 2017). Consumption of excessive amount of energy and natural sources with the large CO<sub>2</sub> emission to the atmosphere led researches to find alternatives, which are sustainable and environmentally friendly, with similar physical properties and chemical composition to Portland cement (Scrivener and Nonat 2011, Yang *et al.* 2008).

Substitution of cement with cementitious materials, which are green, friend to the environment, coming from natural sources and by-products or waste of industrial activities, in cement based materials (Gartner and Hirao 2015) and alkali activation of physically and chemically similar to cement materials are among the most effective ways to reduce CO<sub>2</sub> emission due to cement production.

Roslan *et al.* studied steel slag and sludge as cement replacement in concrete To identify the effect of the admixtures on the concrete they conducted X-ray Fluorescence (XRF) and X-ray Diffraction (XRD) tests.

The result they revealed is that doping of sludge

improves engineering characteristics of concrete and addition of up to 20% steel slag and 15% steel in concrete results strength gain (Roslan *et al.* 2016).

Study of leaching behavior of different type of carbon steel (reinforced bar steel, high alloyed steel and quality steel) slags with respect to their micro structure and crystallographic properties is introduced to the literature by Mombelli *et al.* The study notes that Liquid-on-solid ratio and mineralogical phases in microstructure plays key role on slag leaching characteristics (Mombelli *et al.* 2016).

Coppola *et al.* Investigated the rheological behaviour and mechanical properties of replaced EAFS aggregate concretes in three different sizes. Test results showed that when the ratio of replacement EAFS, elastic modulus, compressive strength and density are also increased but workability is decreased (Coppola *et al.* 2016).

Santamaría-Vicario *et al.* used EAFS and Ladle Furnace Slag (LFS) as replacement aggregate when other mixture materials are constant and searched the durability performance of mortars. According to experimental results, using waste products in mortars increased the durability performance and has good relation between other materials in mortar mixture (Santamaría-Vicario *et al.* 2016).

Traditional alkali activated materials are produced with mixing a precursor which is source of aluminosilicate (fly ash, blast furnace slag, metakaolin and others), alkali activator and fillers (Juenger *et al.* 2011). The precursor in an alkali activated mixture could be waste-stream materials such as fly ash and blast furnace slag and also scrap recycling waste materials (Bajare *et al.* 2014). EAF slag could take place in scrap recycling waste materials due to its sufficient physical properties and chemical composition to be alkali activated.

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Fig. 1 Grinded EAF slag

Electric arc furnace slag (EAF) is a by-product which is produced after the melting and the primary acid refining of liquid steel. EAF needs some primary processes to utilize in concrete or mortar. Firstly, sprinkling and turning, crushing processes are applied and then the artificial aggregate is stored separately according to grain size distribution.

At the end of steel making processes, a great amount of EAF slag landfilled or stockpiled. This, instead, could be used as a cementitious material in mortar or concrete technology due to its amorphous structure and chemical composition. There have been some studies on usage of EAF slag as aggregate (Masoudi *et al.* 2017, Santamaría *et al.* 2017, Faleschini *et al.* 2015) in cement based materials, where the studies suggest EAF slag aggregate sufficiently good to use in cement based materials.

In the current study, alkali activation of EAF is studied with a comprehensive test program. After the investigation of the ANN models' results, ANN and multiple linear regressions based models are compared with each other. After that, an explicit formula is developed with values of the ANN model. In the last part, the effects of silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables are used for the estimation of compressive strength and ANN analysis.

## 2. Experimental studies

### 2.1 Materials

Sodium hydroxide (NaOH), sodium silicate ( $\text{Na}_2\text{SiO}_3$ ) solution, natural aggregate and tap water are used to prepare alkali activated EAF slag mortars. The sodium silicate solution contains 8.52%  $\text{Na}_2\text{O}$ , 27.09%  $\text{SiO}_2$  and 64.39%  $\text{H}_2\text{O}$ . Chemical composition and physical properties of sodium silicate is given in Table 1 and the NaOH used has >99% purity. The aggregate used in the mixture has max 4 mm grain size and having 2.65-2.6 fines modulus and specific gravity respectively. The EAF slag used in the mixtures is gathered from Tosçelik INC. in Iskenderun/Turkey. The EAF slag is pre-crushed firstly and after the pre-crushing process, the size reduction of the EAF slag with the vertical mill crusher is continued. In the vertical mill crusher; the material falls from the feed hopper of the crusher to the rapidly rotating rotator and the material is crushed around the rotor rotating with high speed centrifugal

Table 1 Physical properties and chemical compositions of sodium silicate

Physical and chemical properties	Analysis
( $\text{SiO}_2/\text{Na}_2\text{O}$ )	3.19
Be (at 20°C) (%)	39.40
Density (at 20°C g/cm <sup>3</sup> )	1.37
$\text{Na}_2\text{O}$ (%)	8.52
$\text{SiO}_2$ (%)	27.09
Viscosity (at 20°C, cP)	202

Table 2 Chemical composition of EAF slag (%)

FeO	Fe <sub>2</sub> O <sub>3</sub>	SiO <sub>2</sub>	CaO	Al <sub>2</sub> O <sub>3</sub>	MgO	MnO	K <sub>2</sub> O	TiO <sub>2</sub>	Na <sub>2</sub> O
14.22	17.02	17.04	33.42	11.573	7.62	2.45	0.03	0.04	0.18

force then the collided material collected at the bottom. The EAF slag is broken in abrasive pendulum crusher. The EAF slag is fed to the abrasive pendulum crusher with 3000 kg and 80% of the slag was crumbled to -45  $\mu\text{m}$  fineness. The rotational speed of the pendulum mill is 130 rpm, the mill diameter is 900 mm, the mill rotation speed is 130 rpm, the grinding capacity is 0.5 t/s and the engine power is 18 kWh. After grinding the sample, metals in the slag are separated with using magnetic separators (for the 500 kg slag sample approximately 150 kg metals are separated). Final product has 3.98 g/cm<sup>3</sup> specific gravity and 2600 g/cm<sup>2</sup> blain value. Further, the picture of the grinded EAF slag is illustrated in Fig. 1 and the chemical composition of the sample is given in Table 2. The given chemical compositions of the materials are evaluated by X-Ray Fluorescence (XRF) analysis.

### 2.2 Mix proportioning

72 different mixture were prepared to investigate alkali activation of EAF slag. The design parameters are listed below;

- Three different silicate moduli (1, 1.5 and 2)
- Three different sodium concentrations (4, 6 and 8%) for each silicate moduli
- Two different curing environments (45%-98% relative humidity) for each sodium concentration
- Two different curing temperatures (400C-800C) for each curing environment
- Two different curing times (6h-12h) for each curing temperature

EAF slag: alkali solution: Aggregate ratio was kept constant as 1:2.75:0.485 by mass for all mixtures tested. Detail of the mix proportioning is given in Table 3. To mix the ingredients in the mixtures a speed controlled power-driven revolving pan mixer was used. 10 dm<sup>3</sup> fresh mortar is produced for each mixture. At the beginning aggregate and EAF slag was poured in the mixer and then dry mixed. Then, sodium hydroxide pallets were dissolved in sodium silicate solution. After waiting cooling down of the prepared solution, because the chemical reaction is exothermic, the new solution poured in the dry mixture with water. The mixing continued up to observing a workable mortar. Finally, the mortar was poured in (40×40×160 mm<sup>3</sup>) prisms and vibrated for 30 sec. A day after pouring the mortars, the samples were demolded and

Table 3 Mixture properties and strength values of AAEAFS mortar specimens

Silicate Modulus	Sodium Cons. (%)	RH	Curing Temp.	Curing Time	CS (MPa)	Mix No
1	4	45	40	6	0.60	M1
				12	0.81	M2
			80	6	4.45	M3
				12	7.70	M4
		98	40	6	0.81	M5
				12	1.45	M6
			80	6	7.25	M7
				12	13.59	M8
		45	40	6	4.94	M9
				12	5.58	M10
			80	6	9.25	M11
				12	9.06	M12
	6	45	40	6	5.72	M13
				12	6.38	M14
			80	6	13.34	M15
				12	16.50	M16
		98	40	6	5.73	M17
				12	5.34	M18
			80	6	7.30	M19
				12	7.83	M20
	8	45	40	6	8.00	M21
				12	7.58	M22
			80	6	13.16	M23
				12	16.48	M24
		98	40	6	0.77	M25
				12	1.34	M26
			80	6	6.70	M27
				12	6.78	M28
	4	45	40	6	1.25	M29
				12	2.38	M30
			80	6	10.72	M31
				12	15.70	M32
		98	40	6	4.08	M33
				12	5.22	M34
			80	6	8.95	M35
				12	12.22	M36
1.5	6	45	40	6	5.50	M37
				12	7.20	M38
			80	6	10.20	M39
				12	17.69	M40
		98	40	6	6.27	M41
				12	5.16	M42
			80	6	8.94	M43
				12	14.05	M44
	8	45	40	6	7.23	M45
				12	6.55	M46
			80	6	11.81	M47
				12	17.11	M48

cured under 45%-98% relative humidity for 6h-12h. The presented CS values of each mixture are arithmetic mean value of three specimens.

Table 3 Continued

Silicate Modulus	Sodium Cons. (%)	RH	Curing Temp.	Curing Time	CS (MPa)	Mix No
2	4	45	40	6	1.40	M49
				12	1.56	M50
			80	6	5.28	M51
				12	7.80	M52
		98	40	6	1.78	M53
				12	2.27	M54
			80	6	11.11	M55
				12	18.20	M56
	6	45	40	6	2.34	M57
				12	3.20	M58
			80	6	8.10	M59
				12	12.47	M60
		98	40	6	1.66	M61
				12	2.31	M62
			80	6	12.86	M63
				12	22.02	M64
	8	45	40	6	0.98	M65
				12	1.27	M66
			80	6	5.98	M67
				12	8.38	M68
		98	40	6	1.36	M69
				12	1.81	M70
			80	6	10.83	M71
				12	16.88	M72

### 2.3 Test methods

Three different silicate moduli (1-1.5-2), three different sodium concentrations (4%-6%-8%) for each silicate module, two different curing conditions (45%-98% relative humidity) for each sodium concentration, two different curing temperatures (400°C-800°C) for each relative humidity condition and two different curing time (6h-12h) for each curing temperature variables are selected and their effects on compressive strength was evaluated. Then the regression equations using multiple linear regressions methods are fitted. These multiple linear regression methods contain linear, interaction, quadratic and pure quadratic models. And then to select the best regression models confirm with using silicate moduli (SM), sodium concentration (SC), relative humidity (RH), curing temperature (CE) and curing time (CT) variables, the regression models compared between itself using mean square error (MPE), correlation coefficients ( $R^2$ ), mean square error (MSE) criteria. In the following section, information about the ANN method is given. In the following parts of the article the ANN (Artificial Neural Network) models that use silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables, are formed.

Compressive strength tests were performed on 40×40×40 mm<sup>3</sup> cubes by a 2500 kN compression capacity testing machine according ASTM C349.

### 3. Multiple linear regression methods for estimation of compressive strength

The regression equations are the formulization of the relationship between dependent and independent variables. These equations aims in this section to estimate the dependent variable which is the compressive strength using the independent variables which are the silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables at the base of multiple linear regressions. Multiple linear regression models are built from a potentially large number of predictive terms according to independent variables. Each model has different number of coefficients. Coefficients of multiple linear regressions models are determined according to 72 different experimental data for estimation of compressive strength in this study. The terms produced from the variables are highly effective in increasing the accuracy of estimates. For example, the number of interaction terms increases exponentially with the number of predictor variables. If there is no theoretical basis for choosing the form of a model, and no assessment of correlations among terms, it is possible to include unnecessary terms in a model that confuse the identification of significant effects. Multiple linear regression models often take the form of Something like Eq. (1)

$$y(x) = \beta_0 + \sum_{i=0}^N \beta_i x_i + \sum_{i < j}^N \beta_{ij} x_i x_j + \sum_{i=0}^N \beta_{ii} x_i^2 + \varepsilon \quad (1)$$

In this formula,  $x_i$  ( $i=1, \dots, N$ ) represents independent variables,  $y$  represents dependent variable,  $\beta$  represents coefficients of regression,  $\varepsilon$  represents error. A response variable  $y$  is modeled as a combination of constant, linear, interaction, and quadratic terms formed from predictor variables  $x_i$ . Uncontrolled factors and experimental errors are modeled by  $\varepsilon$ . The regression estimates model coefficients.

With the multiple linear regression approach, linear additive model, pairwise interaction model, quadratic model and pure quadratic model are formed in MATLAB program by experimental data set. The experimental data set consisting of 72 experiments is used to determine the coefficients of the regressions formulas.

The data set is divided into two parts as calibration and test in order to prevent overfitting of models. The calibration data set consists of 80% of the data. The test data set consists of the remaining 20%. With the calibration data set, MLR models fit. With the test data set, it is checked whether the fitted MLR models are overfitted. The formula of linear additive model based on multiple linear regressions is shown in Eq. (2).

$$CS = -15.4497 - 0.9181 * SM + 0.5848 * SC + 0.0693 * RH + 0.1959 * CE + 0.43475 * CT \quad (2)$$

In this formula, CS, SM, SC, RH, CE and CT letters stand for compressive strength, sodium moduli, sodium concentration, relative humidity, curing temperature and curing time, respectively. Pairwise interaction model based on multiple linear regression has a formula which is shown in Eq. (3)

$$\begin{aligned} CS = & 5.1583 - 2.5313 * SM + 3.1487 * SC - 0.1397 \\ & * RH - 0.2236 * CE - 1.0857 * CT - 1.0735 * SM \\ & * SC + 0.0041 * SM * RH + 0.0971 * SM * CE \\ & + 0.2299 * SM * CT + 0.00077 * SC * RH - 0.0095 \\ & * SC * CE - 0.0448 * SC * CT + 0.0025 * RH * CE \\ & + 0.0056 * RH * CT + 0.0167 * CE * CT \end{aligned} \quad (3)$$

Quadratic model based on multiple linear regression has a lot of terms about five independent variables. These terms take part in Eq. (4)

$$\begin{aligned} CS = & 730290190602419 + 6.9334 * SM + 8.1380 \\ & * SC - 5047207384746.1 * RH - 21238285812614.3 \\ & * CE + 234884742242.87 * CT - 0.9525 * SM * SC \\ & + 0.0075 * SM * RH + 0.0998 * SM * CE + 0.2483 \\ & * SM * CT + 0.00022 * SC * RH - 0.0091 * SC * CE \\ & - 0.0373 * SC * CT + 0.0024 * RH * CE + 0.0059 \\ & * RH * CT + 0.0160 * CE * CT - 3.6369 * SM^2 \\ & - 0.4358 * SC^2 - 34334744114 * RH^2 \\ & + 176985715105 * CE^2 - 13049152347 * CT^2 \end{aligned} \quad (4)$$

The formula of pure quadratic model based on multiple linear regression is shown in Eq. (5)

$$\begin{aligned} CS = & 2274156745834820 + 6.0487 * SM + 6.0567 \\ & * SC + 896714760127 * RH - 59114541019104 \\ & * CE - 181765416872386 * CT - 2.4266 * SM^2 \\ & - 0.4598 * SC^2 - 61001100409 * RH^2 \\ & + 492621175159 * CE^2 \\ & + 100908078715132.6 * CT^2 \end{aligned} \quad (5)$$

After the regression analyses, the models are compared with the performance criteria which are correlation coefficient, mean percent error and mean square error used in this study. These methods on error comparison are very useful for finding the best models. The correlation coefficient is used to understand the correlation between the results of the models and the experimental values. The mean percent error criterion is calculated to take into consideration the error ratio according to each experimental which has small or big value of compressive strength. Another criterion to find the best model in this study is the mean square error (MSE) which was used to evaluate the performances of the models.

According to calibration and validation data sets,  $R$ , MSE and MPE values of the models are determined. So whether the models are overfitted or not is checked. As shown in Table 4, the  $R$ , MSE and MPE values of the calibration and validation data sets are close to each other. Thus, it is understood that the models do not overfit. It is

Table 4 Comparison of multiple linear regression methods for estimation of compressive strength

MLR Models	Calibration			Validation		
	$R$	MSE	MPE (%)	$R$	MSE	MPE (%)
Linear model	0.674	9.6872	63.22	0.68	9.7537	65.98
Interaction model	0.843	3.6426	39.48	0.826	4.4274	37.52
Quadratic model	0.892	2.3144	20.13	0.903	2.4769	25.04
PureQuadratic model	0.776	8.7539	57.61	0.779	9.1346	55.49

Table 5 Correlation matrix values between compressive strength and other terms

	SM	SC	RH	CE	CT	SM*SC	SM*RH	SM*CE	SM*CT	SC*RH
SC	-0.05618	0.212214	0.32025	0.751438	0.218808	0.080351	0.209764	0.565394	0.142458	0.374236
	SC*CE	SC*CT	RH*CE	RH*CT	CE*CT	SM <sup>2</sup>	SC <sup>2</sup>	RH <sup>2</sup>	CE <sup>2</sup>	CT <sup>2</sup>
SC	0.689007	0.292654	0.792961	0.3919	0.709325	-0.06448	0.195572	0.32025	0.751438	0.218808

seen that the quadratic model is the best model to estimate compressive strength when the multiple linear regression methods are compared (Table 4. Performance criteria for the estimation of the results of quadratic model are as follows: correlation coefficient 0.892, mean square error 2.3144, mean percent error 20.13%.

However, the Quadratic Model, which is the best MLR model, can be simplified by subtracting terms with little effect. Thus, an effective equation that is easy to use can be obtained. For this purpose, the terms of SM, SM \* SC, SM \* RH, SM \* CE, SC \* RH, SC \* CE, RH \* CE, RH \* CT, CE \* CT and SM<sup>2</sup> have been eliminated by considering the correlation analysis and regression analysis. Because these terms have little effect (Table 5). When the terms with little effect are excluded, the following simple and effective equation is obtained (Eq. (6))

$$\begin{aligned}
 CS = & -474598130998371 + 8,38 * SC \\
 & + 12423700058819 * RH - 6336894264214 * CE \\
 & + 59435277363991 * CT + 0,25 * SM * CT \pm 0,02 \quad (6) \\
 & * SC * CT - 0,45 * SC^2 - 84514966387 * RH^2 \\
 & + 52807452202 * CE^2 - 3301959853555 * CT^2
 \end{aligned}$$

#### 4. The artificial neural network

Many complex issues faced by engineers are solved easily thanks to the advantages of the ANN method, and the indefinable relations between variables are reflected in the results. As a result, more successful results can be reached with the ANN method than those of statistical methods. Besides, models can be developed with the ANN method, which is developed on the basis of a biological neuro-system, without any pre-condition, as opposed to statistical methods. If enough data is provided, quick and practical estimation models can be formed using the ANN method. Besides, raw data is examined with statistical analyses and data evaluation is realized before the formation of the ANN method.

The ANN method has powerful mathematical instruments that can form non-linear connections between inputs and outputs. The dissemination of every input with different weights to the neurons on the next layer, to process these inputs through transfer functions after gathering and re-dissemination of these inputs with different weights to the next layer, shows that inputs are being processed by a number of mathematical instruments in the network. Apparently, the most attractive part of the ANN method is its highly developed learning capability. Learning, which means to determine the weights among neurons, is realized through intense mathematical algorithms.

In the ANN method, models like black box are formed without knowing the complex connections between

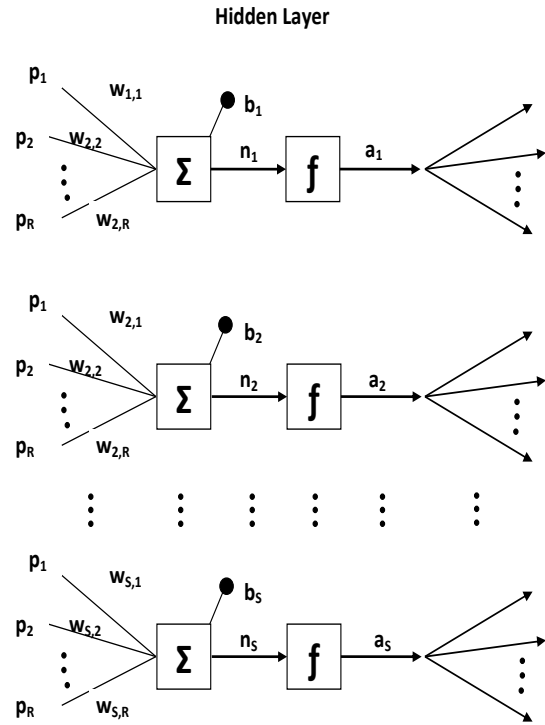


Fig. 2 A hidden layer of a network with  $R$  input elements and  $S$  neurons (according to Matlab notations)

variables (Karayiannis and Venetsanopoulos 1993). To explain, models are formed without depending upon engineering determinations and settling analytical bases for connections between inputs and outputs. Reaching results like black box without intervening in the processes in the network is a disadvantage of the ANN method. Another significant disadvantage of the ANN method is learning by heart. If there are immense mistakes in test outputs in spite of excellent outputs in train outputs, the ANN method is not learning, but actually memorizing. To avoid this circumstance, it is essential to form the best model by controlling the error ratings in the train, validation and test data.

The ANN is formed by layers of artificial neurons. Inputs from former layer are accumulated by multiplying with weights and bias is added. The results of artificial neurons are then determined by processing this accumulation through the transfer function Eq. (7). This result is disseminated to the latter layer by multiplying with weights in Fig. 2.

$$a_s = f\left(\sum w_{sR}p_R + b\right) \quad (7)$$

In this formula,  $a$  represents the result of the artificial neuron,  $w$  represents the connection factor (weight) between neurons,  $p$  represents the inputs coming from the former

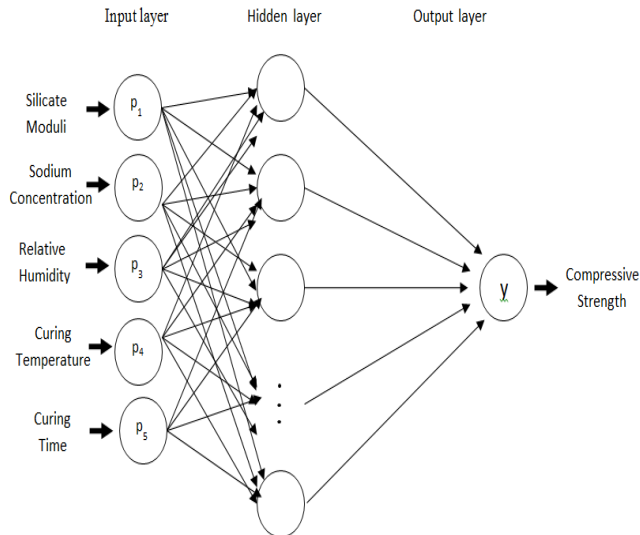


Fig. 3 A feed forward neural network for estimating compressive strength

layers,  $f$  represents the transfer function,  $b$  represents the bias,  $S$  stands for the number of neurons and  $R$  stands for the input number (MATLAB).

The layers made by artificial neurons are in three sections. When the first section is input layer, the second section is hidden layer. The last section is output layer. Despite the fact that there are no connections between the neurons in a layer, connections are formed with the neurons in the former and latter layers.

Establishing the optimum layer number and optimum neuron number is important in order to achieve the best results. Moreover, the higher number of layers and neurons can produce undesired results. Generally, ANN models with single hidden layer are used in engineering problems (Saridemir 2008, Arslan 2009, Demirci 2013). The optimum neuron number is determined according to best results with the empirical methods. A feed-forward ANN method, which is made up of a single hidden layer and an output layer, is shown in Fig. 3.

The value of weights which form the connection between neurons is determined with the train process. By changing the value of weights according to number of errors between input and output values, the best weights are achieved in every phase of training. In fact, to determining the weighted rating is a study of optimization.

The results of this research show that predicting the compressive strength needs only one hidden layer. To determine the fittest ANN structure to forecast the compressive strength, various ANN structure were constructed and trained. During the construction of the ANN model, the neuron number was varied from 1 to 25 in the second layer. The most used Matlab training algorithms (GD, GDM, LM, RP) were used for the training of the ANN structures. The linear transfer function called Purelin was applied in the model. S-shaped tan-sig and log-sig transfer functions were used in the ANN structures. In comparison of the models, MSE value is employed for performance criteria.

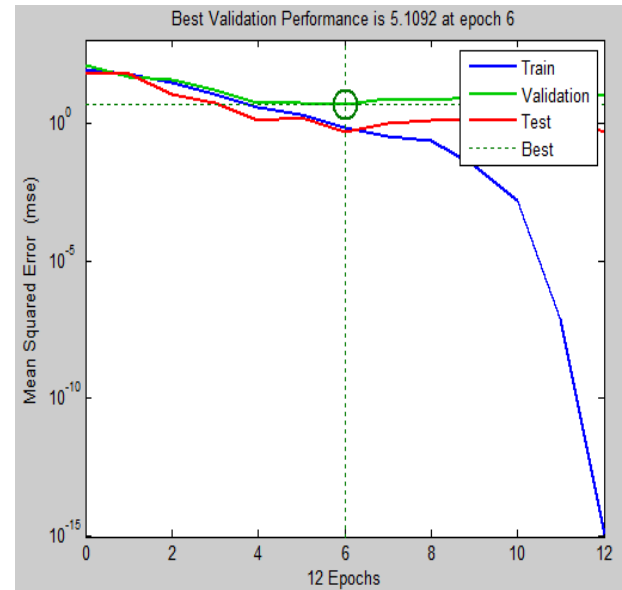


Fig. 4 Training process of ANN model

## 5. The formation of the ANN model for estimation compressive strength

The ANN model is developed the ANN method. The ANN model has the variables of silicate moduli, sodium concentration, relative humidity, curing temperature and curing time in input layer. The ANN model is trained with the train and validation data set randomly selected from 72 experiments results. While the train and validation data set been formed 58 and 7 experiments results respectively, the test data set confirmed 7 experiments results. Therefore, one of the major drawbacks of ANN, which is to find appropriate train data, was eliminated.

While in a single hidden layer the ANN model which has 19 neurons, the tansig transfer function, the output layer has one neuron and purelin transfer function. Levenberg-Marquardt train algorithm produces the best results for the prediction of compressive strength in the ANN model. Fig. 4 presents the mean square error values of ANN model depend on the epoch number for the train, validation and test sets. The best line shown on Fig. 3 illustrates start point of the overfitting. In this study, with aid of maximum validation failures criteria, training process of the ANN model was ended. In the Matlab, it was accepted that when the MSE values of the train and validation sets are decreasing simultaneously, it shows the learning process continues, however, the MSE values of training set continues to while the MSE values of validation set tend to increase, the training process stopped. Training stopped when the validation error increased for six iterations, in this study as seen on Fig. 4 training stooped at iteration 12. Fig. 3 also presents the result is reasonable because of the following considerations:

- The final mean-square error is small.
- The test set error and the validation set error has similar characteristics.
- No significant overfitting has occurred by iteration 6 (where the best validation performance occurs).



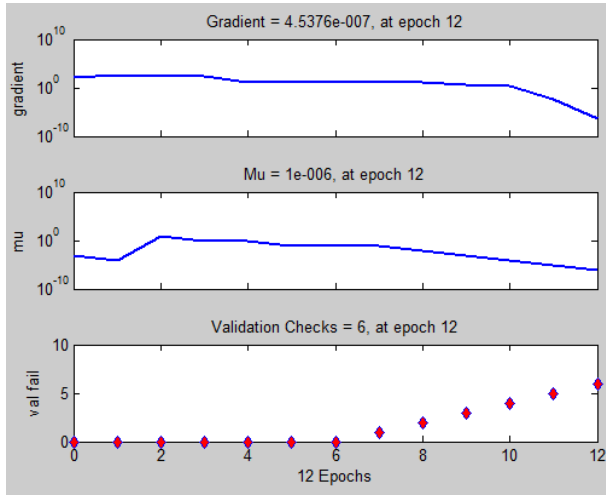


Fig. 5 Changing of parameters at training process of ANN

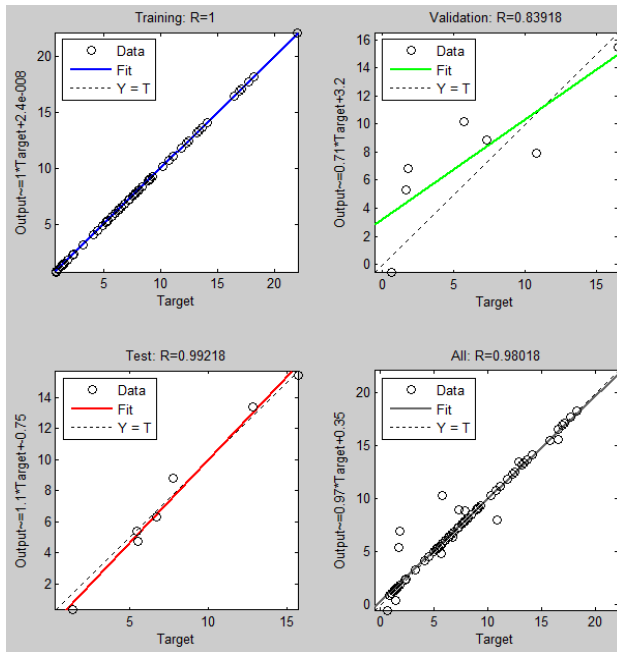


Fig. 6 Comparison of outputs of ANN between targets

When looked at the ANN model statistical parameters after completing the training process, it is observed that it has 5.1092 Validation MSE at epoch 6. Train, validation and test sets MSE values of ANN model are illustrated in Fig. 4.

Fig. 5 shows changing of gradient, mu and validation failure of training set according to epoch number. Gradient value changed between 350.9534 and 0.00000045376. Value of mu increased from 0.000001 to 10. Because of the validation failure occurred at the iteration 12, training process stopped and no significant overfitting has occurred by iteration 6 where the best validation performance occurs.

Fig. 6 presents the training, validation, test and all data sets correlation performances between outputs of ANN and targets values.  $R$  of train and test data sets are very close to each other. Correlation consistency among the three data sets is a good evidence of how the ANN model well trained. Taking into account the all data,  $R$  was as high as 0.98018.

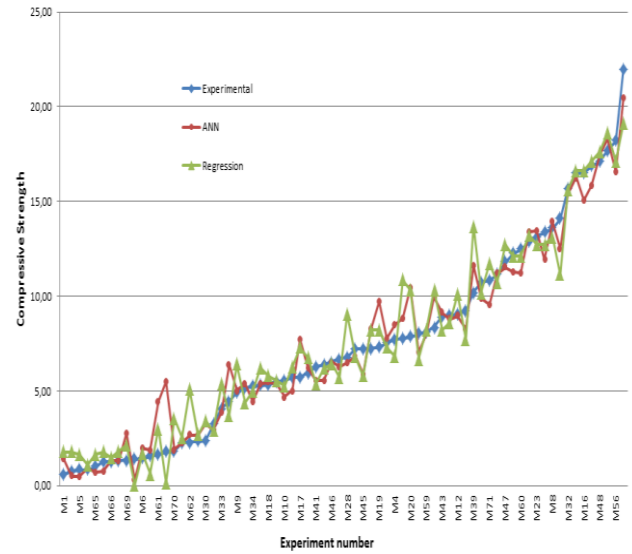


Fig. 7 Comparison of experimental, regression and ANN model results

## 6. Comparison of regression and ANN with models

When the quadratic model based on multiple linear regression approach is compared with ANN model using the ANN method, on the whole data set. MSE of the ANN model is less than Regression Model (Table 6). Likewise, while the Regression model has 0.895  $R$  value, the ANN model has 0.98. When we look at the MPE value, the ANN model again has a better value of 20.32% compared to 22.48% in the Regression model. The effects of value in experimental phase or the harmonious movement with the ANN curve and experimental values can be seen in Fig. 7.

## 7. ANN model based explicit formulation

In this section, an explicit formula was developed with values of the ANN model. The formula has the transfer function, weights and bias of the ANN structure. The compressive strength is the function of silicate moduli, sodium concentration, relative humidity, curing temperature and curing time defined in Eq. (8)

$$\text{tansig} \left( \begin{matrix} \text{CS} = \text{purelin} \\ \begin{matrix} 1.581799 & 2.365208 & 0.261874 & -0.2564 & -0.10819 \\ -1.55383 & 0.95945 & -2.02787 & 0.061235 & -1.31533 \\ -1.16401 & 1.151355 & -1.05224 & 2.280118 & -0.32605 \\ -0.41215 & -0.90278 & -1.84492 & -1.78111 & 0.686432 \\ -0.81286 & -1.69069 & -0.86655 & 1.125644 & 1.727874 \\ -1.97238 & -0.0947 & -0.70962 & 1.793268 & -1.0356 \\ 1.369151 & 1.418379 & 0.145962 & 2.677961 & 0.17453 \\ -1.7412 & 2.110601 & 1.007521 & 1.26828 & -0.30693 \\ -1.59762 & -1.25883 & -0.44285 & -0.83865 & 1.96035 \\ 0.127881 & 0.830983 & -0.18809 & 1.167769 & 0.996511 \\ 0.95253 & 0.212781 & -1.2955 & -1.22346 & 1.812342 \\ -1.7533 & -0.77291 & 1.517695 & 0.285937 & -1.65716 \\ -0.08648 & 0.467353 & 0.353096 & 2.165038 & 1.488771 \\ 0.936431 & 1.046818 & 0.27427 & 0.282678 & 2.537904 \\ -3.10568 & -1.60471 & 0.156212 & -2.19328 & -0.70212 \\ -1.52056 & -1.53646 & -0.14186 & 1.706537 & -1.09303 \\ -0.43146 & -1.56041 & 0.996062 & -1.97337 & -1.3031 \\ 0.016545 & 0.741542 & -1.76791 & -0.42858 & -1.95968 \\ 2.338076 & -0.17697 & -1.45646 & -1.45646 & 0.829682 \end{matrix} \end{matrix} \right)$$

$$\begin{matrix}
 \begin{bmatrix} SM \\ SC \\ RH \\ CE \\ CT \end{bmatrix} \\
 * \\
 \begin{bmatrix} -2.90804 \\ 2.17984 \\ 2.643366 \\ 1.91615 \\ 1.371416 \\ 2.178009 \\ -1.35846 \\ 1.411163 \\ -0.2466 \\ -0.50581 \\ 0.177755 \\ -0.18864 \\ -1.49166 \\ 0.709458 \\ -0.07468 \\ -1.06052 \\ -1.80429 \\ 2.423187 \\ 2.023863 \end{bmatrix} \\
 + + \\
 \begin{bmatrix} 2.275272 \\ 0.562123 \\ -2.06916 \\ 0.808249 \\ -0.23602 \\ 2.050767 \\ -0.92052 \\ -1.19253 \\ 0.567452 \\ 0.098054 \\ 0.754038 \\ -0.33382 \\ -2.48185 \\ 0.479345 \\ -0.63875 \\ 0.850673 \\ 0.889622 \\ 0.456143 \\ -0.63764 \end{bmatrix} \\
 + [0.082224]
 \end{matrix} \quad (8)$$

In Eq. (7), SM stands for the silicate moduli, SD stands for the sodium concentration, RH stands for the relative humidity, CE stands for the curing temperature CT stands for the curing time, CS stands for the compressive strength,  $T$  represents transpose, tansig stands for tangent sigmoid transfer function (Eq. (9)), purelin stands for linear transfer function (Eq. (10)).

$$tansig(n) = \frac{2}{(1 + \exp(-2 * n))^{-1}} \quad (9)$$

$$purelin(n)=n \quad (10)$$

In Eqs. (9)-(10),  $n$  represent the result of related process of weights and bias. The variables were normalized to a range of (-1,1) by Eq. (11). The maximum and minimum values of variables were demonstrated in Table 7.

$$\frac{(y_{\max} - y_{\min}) * (x_{\max} - x_{\min})}{x_{\max} - x_{\min}} \quad (11)$$

## 8. Results of the models

In this article, regression method's and ANN method's abilities in estimating the compressive strength with the silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables, are compared

Table 6 Comparison of  $R^2$ , MSE and MPE of experimental, regression and ANN model results

	$R$	MSE	MPE
Regression	0.895	2.34	% 22.48
ANN	0.980	1.12	% 20.32

Table 7 Range of input and output parameters

Variable	Max	Min
Compressive Strength	22.02	0.6
Silicate Moduli	2	1
Sodium Concentration	8	4
Relative Humidity	98	44
Curing Temperature	80	40
Curing Time	12	6

with different and similar aspects.

When the correlation analysis is considered, it is understood that the curing temperature variable is very related to the compressive strength variable. However, relative humidity, curing time, and sodium concentration seem to be related to the degree of significance. The silicate moduli variable appears to be less related to the negative direction. When we look at the regression analysis, it is seen that the relative humidity, curing temperature and curing time variables of the independent variables are very effective on the dependent variable of compressive strength. Silicate moduli and sodium concentration independent variables are relatively less effective.

In comparing with linear, interaction, quadratic and purequadratic models, which are constructed with multiple linear regression approach, the quadratic model provides better results. With developing quadratic regression model, MPE declined to 22.48%,  $R$  rose to 0.895. The MSE value, which is a very important criterion for comparing model results became less than 2.34 and positive developments are seen in the whole evaluation criteria. Similarly, from the models that are based on the ANN method the ANN model using nineteen neurons in the hidden layer rather than the other neuron number in the hidden layer provides the best result. With the ANN model, the  $R$  rose to 0.98, the MPE declined to 20.32%, while the important criterion of MSE, which shows high performance in model comparisons declined to 1.12. When comparing the MLR model which is the best among the regression based models and the ANN with nineteen neurons in the hidden layer which is the best in ANN based model, the results of the ANN based model are superior. In estimating the compressive strength ANN methods show better performance than the multi linear regression methods.

## 9. Conclusions

According to outcomes, the under mentioned conclusions can be drawn:

- The quadratic model based on multiple linear regression contains silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables and the quadratic model was fitted all of the data set. The MLR model has 0.895, 2.34, 22.48% correlation coefficient, MSE and MPE values, respectively.
- The results of improved ANN model compare with quadratic model, it is seen that the ANN model has better results than the quadratic model with 0.98  $R$ , 1.12 MSE and 20.32 % MPE values.
- The ANN model consisted with silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables, one hidden layer, 19 neurons in the hidden layer, has the best performance values with correlation coefficient of 0.98, MSE of 1.12 and MPE of 20.32% values for the estimation of compressive strength.
- The fluctuations of data set of the compressive strength were very well reflected using ANN models constituted



silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables. Furthermore, the ANN models gave better reflection than the multiple linear regression models.

- It has an incentive effect for future studies to know that both of the methods, multiple linear regression with quadratic terms and ANN, produce better results to estimate compressive strength using silicate moduli, sodium concentration, relative humidity, curing temperature and curing time variables.

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