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A Predictive Model Based ANN for Compressive Strength Assessment of the Mortars Containing Metakaolin

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ABSTRACT

A predictive model based on the artificial neural network (ANN) was generated to assess the compressive strength of Mortar incorporating metakaolin (MK). For this purpose, a database was gathered from different works of literature for use in the ANN model. Therefore, five predictive variables as the inputs of the ANN model were considered, including the age of the samples, the ratio of MK replacement, the ratio of water to the binder, the ratio of superplasticizer, and the ratio of binder to sand. Using the constructed ANN model, a new formula has been presented, which can predict the compressive strength of the mortars incorporating MK. Then, the performance of the presented formulae was examined. The obtained conclusions indicated that the evaluated formula can predict the compressive strength of the mortars containing MK. Also, in the end, Garson's algorithm as a sensitivity algorithm was employed to examine the effect of each predictive variable on the compressive strength of the mortars incorporating MK. The results reveal that the binder-sand ratio is a more important parameter in determining the compressive strength of the mortars incorporating MK.

1. Introduction

The use of pozzolan in concrete and mortar shows a significant modification in their properties. Recently, the addition of MK as a form of calcined clay for mortar and concrete has received

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great attention. The MK obtained from calcining kaolin as a thermal procedure by heating ranging from 700-850 °C. The two important reasons to use this type of pozzolans are material durability and accessibility. Also, the use of filler and accelerated cement hydration together causes early increasing of strength in mortar and concrete. Furthermore, the shrinkage in the concrete with MK (up to 15%) replacing by cement is less than concrete without MK [1–5]. To date, several studies have been accomplished which pointed increasing the compressive strength (f_c) of the concrete or mortar with MK, specifically at the initial curing time. Two groups of specimens with 36 mixes were made by Vu et al. [6]. In the first group by 6 mixes the binder to sand ratio was 1:2.75, while in the second group by 30 mixes, the binder to sand ratio was 1:2. Five values of MK were considered for these mixes including 10, 15, 20, 25 and 30 percent of MK replacing by cement weight and also one mix without MK was considered as the control mix. They found that f_c of the mortars with 10%, 15% and 20% MK replacing as cement increased at 7, 28, 60 and 90 days. Also, for the mixes by 30% MK replacement, f_c of mortars decreased at 7, 28, 60 and 90 days. Parande et al. [7] replaced cement by MK in mortar specimens in the ratios of 5%, 10%, 15%, and 20%. These specimens include the ratio water to cement 0.40 and the ratio of binder to the sand of 1:3. They found that f_c of the mortars with MK was increased until the end of 90 days. Also, it was found that the best outcomes were related to the specimens with 15% MK. In another research, Courard et al. [8] reported specimens with 10%, 15%, 20%, 25%, and 30% MK replacing as cement weight. They also used the mixes without any mineral admixture to control these specimens. They found that f_c of the specimens with 15% MK yielded the maximum values, while the age of specimens was 2, 7, 14 and 28 days. Here, the ANN is applied for estimating the f_c in the mortars containing MK. The ANN as a type of artificial intelligence was applied for input-output models. In these models, experimental or numerical datasets (according to experimental or numerical studies) are used for training the system. If by using the database, appropriate information is obtained about the problem, therefore the trained ANN model will contain sufficient information about the response and the model can be qualified as a reliable model. In the previous papers, artificial intelligence including ANN has been used for different applications in engineering, including assessment of the ultimate capacity of beams [9–22], evaluation of compressive strength in columns [23,24], prediction of permanent earthquake-induced deformation [25], assessing compressive strength of geopolymer stabilized clayey soil [26], prediction of compressive strength in concrete or mortar [27,28], etc.

2. Experimental dataset

In this article, the experimental dataset including 176 specimens was obtained from reliable literature [6–8] for using in the ANN model. Generally, the compressive strength of the mortars incorporating the MK may be related to the age of samples (AS), percentage of the replacing metakaolin ($MK\%$), ratio of water-binder (WB), percentage of the used superplasticizer ($SP\%$) and also ratio of binder-sand (BS); therefore, all the effective parameters were considered in this study to examine the efficacy of them for evaluating the f_c of the mortars incorporating the MK. The statistics of these variables applied in the ANN structure are measured and tabulated in Table 1. Moreover, to illustrate the distribution of the used variables histograms for frequency calculated and the results shown in Fig. 1.

Table 1
The statistics performance for used variables.

Parameter	AS	MK	WB	SP	BS	f_c
Mean	38.9239	14.3478	0.4733	0.1783	0.4393	38.7543
Std. Error of Mean	2.41431	0.62187	0.00332	0.02842	0.00563	1.00853
Median	28.0000	15.0000	0.4800	0.0000	0.5000	42.1000
Std. Deviation	32.74933	8.43546	0.04504	0.38548	0.07643	13.68036
Variance	1072.519	71.157	0.002	0.149	0.006	187.152
Range	89.00	30.00	0.13	1.30	0.17	69.05
Minimum	1.00	0.00	0.40	0.00	0.33	2.15
Maximum	90.00	30.00	0.53	1.30	0.50	71.20

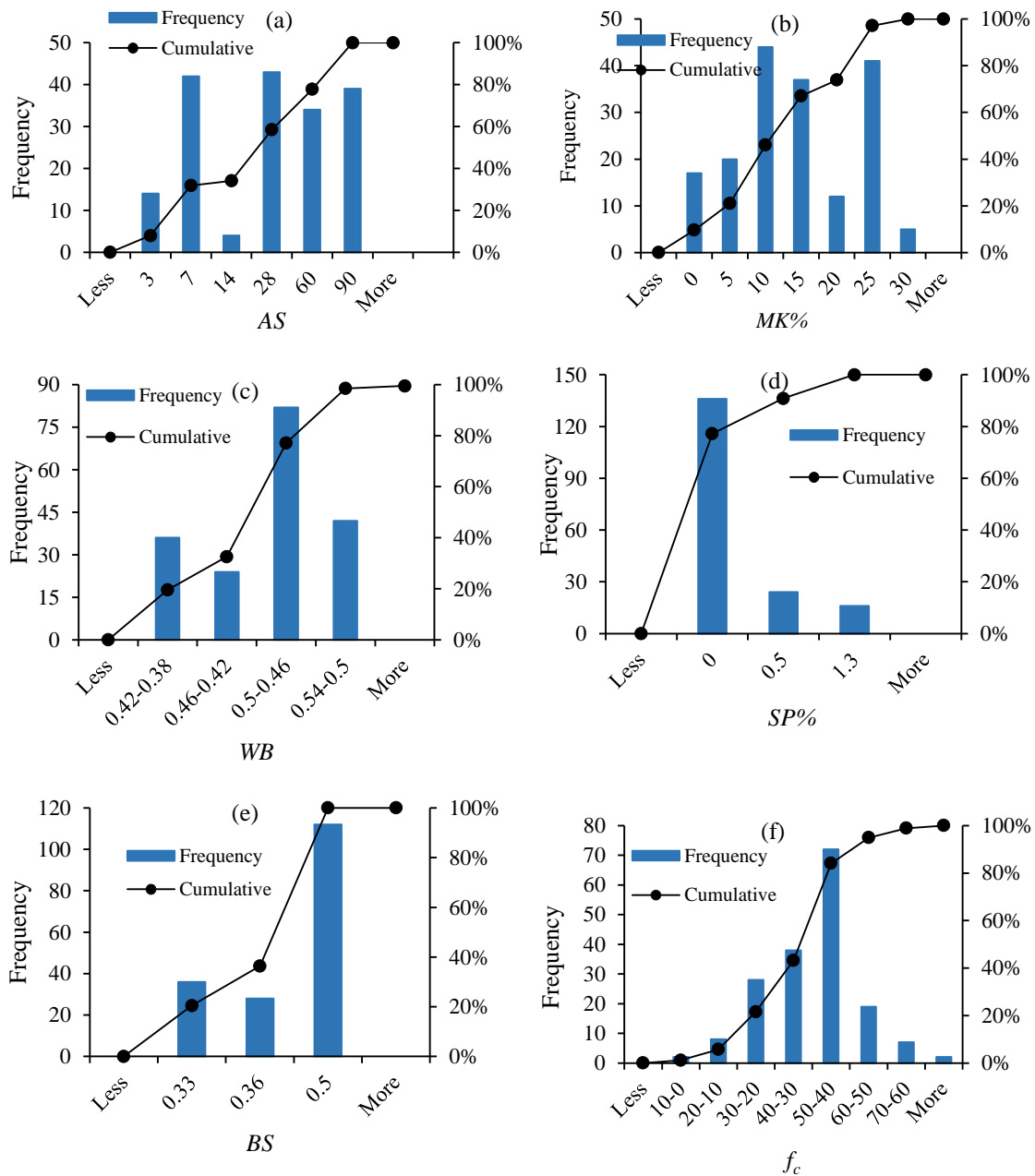


Fig. 1. Frequency histograms of the variables.

3. Artificial neural network (ANN)

The ANN method is a branch of soft computing theory that employed the organization of the biological neural networks. Here, the ANN model was applied to derive new practical formulation for the compressive strength of the mortars containing MK. As a result, the relationship between the influencing variables on the compressive strength of the mortars containing MK was attained using an efficient ANN procedure training. The multilayer perceptron (MLP) is one of the training methods that are more efficient while using a feed-forward scenario. The aforementioned network development is applied suitable for any continuous function to an arbitrary grade of precision [27,28]. The feed-forward procedure is based on evaluating the output/s using dependent or independent input variables. As it can be found the feed-forward procedure flow forward from first to last layers without the feedback loop (See Fig. 2). Each layer in the feed-forward procedure connects to synapses, consequently, a weight that presents the influence of the neuron is connected to synapses.

The back-propagation (BP) algorithm is a supervised learning procedure which applied for multilayered networks. This algorithm is considered by a procedure in which a specified output is compared to the expected output so that the weights would be adapted based on this comparison. Until the model error is converged to the specified performance function, the BP algorithm is minimized. A trial and error procedure is being carried out to develop the structure of the ANN. Each input signal is attached to its corresponding weight and then is added to a bias. Finally, the outcome is estimated through an activation function the input of each node is presented as below:

$$net_j = \sum_{i=1}^n w_{ij}x_i + b_j \quad (1)$$

where net_j is the set of data from each neuron and x_i , b_j and w_{ij} specify the input value, the bias value and the related weight value, respectively. Neuron output is evaluated using transfer function that employed to involve nonlinearity into ANN. Implementation of the nonlinearity mechanism improves the accuracy of the ANN developed program. The relevant transfer functions are as Sigmoid, Hyperbolic tangent and Gaussian functions. Therefore, the outputs function may be presented as:

$$out_j = f(net_j) \quad (2)$$

where out_j and f are the output of the j th neuron and transfer function, respectively. Fig. 2 depicts the arrangement of a typical ANN.

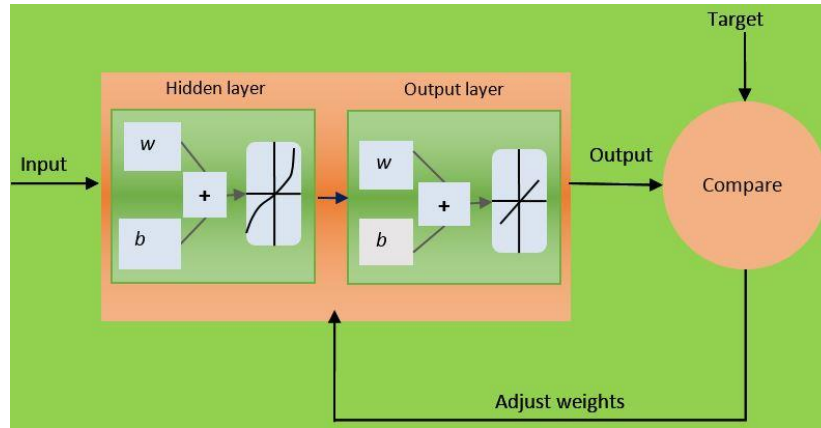


Fig. 2. Arrangement of simple artificial neural networks.

3.1. Performance measures

In this study, four measures are applied in order to investigate the ANN model efficiency as absolute percentage error (Err), mean absolute error (MAE), mean squared error (MSE) and correlation coefficient (R). The above-mentioned criteria can be presented as below:

$$Err_i = \frac{|y_i - t_i|}{t_i} \times 100 \quad (3)$$

$$MAE = \frac{1}{N} \sum_{i=1}^N |y_i - t_i| \quad (4)$$

$$MSE = \frac{1}{N} \sum_{i=1}^N (t_i - y_i)^2 \quad (5)$$

$$R = \frac{\sum_{i=1}^N (y_i - \bar{y}_i)(t_i - \bar{t}_i)}{\sqrt{\sum_{i=1}^N (y_i - \bar{y}_i)^2 \sum_{i=1}^N (t_i - \bar{t}_i)^2}} \quad (6)$$

where N shows the number of samples, t_i and \bar{t}_i indicate the exact output and the average of the exact output, respectively, and y_i and \bar{y}_i present the examined output and the average of the examined output, respectively.

3.2. ANN structure for predicting f_c

The Levenberg-Marquardt (LM) algorithm [29] is generated for training the ANN. The LM algorithm converges in fewer epochs than other learning algorithms. Each epoch presents one forward and one backward pass of all training samples. The LM algorithm can converge the training process with few hundred weights [30]. The recognition of the parameters which affect the f_c is difficult and the effective parameters are not independent of each other and some of them may be strongly related together. As mentioned, the initial variables for the ANN were chosen as below:

$$\text{Input} = \{AS, MK \%, SP \%, WB, BS\}$$

$$\text{Output} = \{f_c\}$$

The number of hidden neurons affects the accuracy of the output. A trial-and-error algorithm was generated to find the optimized numbers of neurons. Each network by more neurons in the hidden layer yields a tedious and lengthy equation. Therefore by considering the accuracy of the model, in the current paper, a model by three nodes is considered. The used data in the training state is an important problem and it is mainly related to the reliability of the model [31]. Frank and Todeschini [32] discussed that the minimum ratio of the entire to input variables numbers for the acceptability of the model is three. Moreover, they recommended a ratio of five to obtain a more strongly model. Here, the mentioned ratio was equal to $176/5 = 35.2$. The Log-Sigmoid transfer function was applied in both hidden and output layers to derive the formula in explicit form. The predicted results of f_c values by the ANN model are illustrated in Fig. 3. It is shown in Fig. 3 that training, validation and testing data sets yield a good correlation between actual and predicted values.

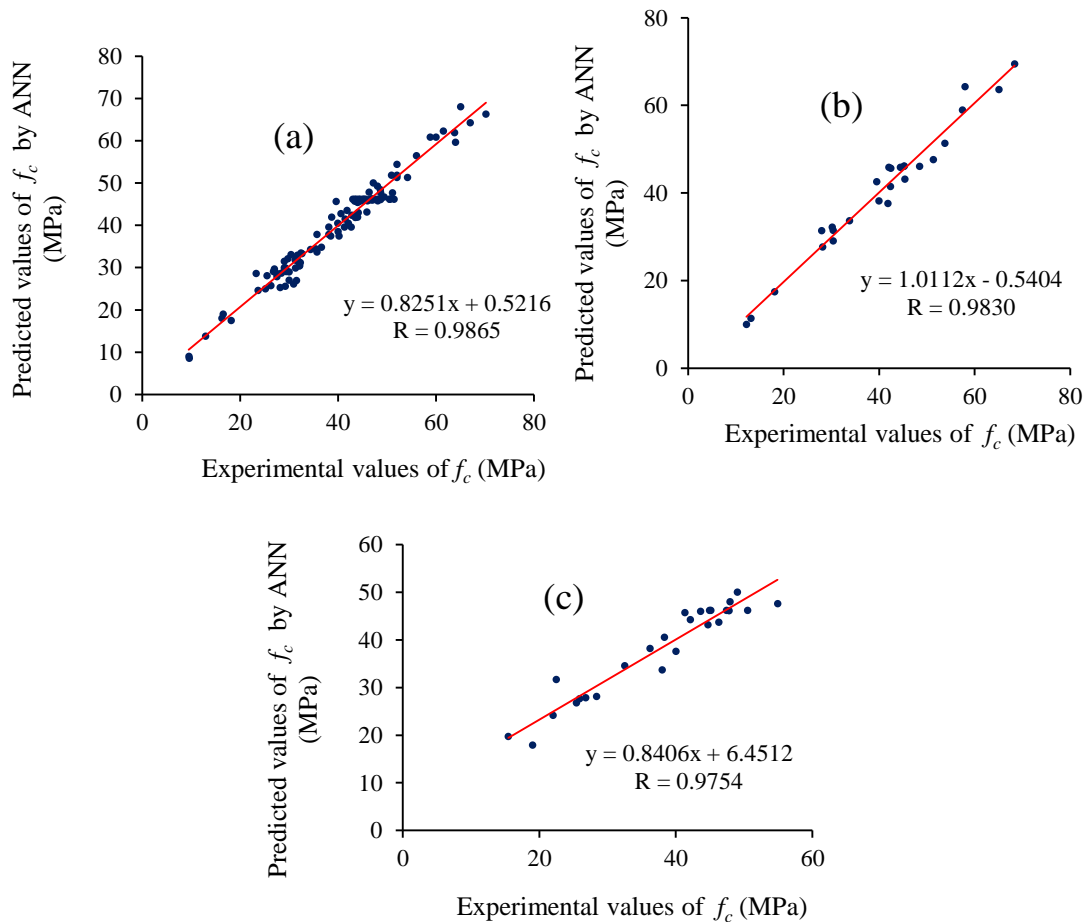


Fig. 3. The output predictions based on the ANN model. (a) Training data, (b) validation data and (c) testing data.

3.3. Empirical formula development

The output of each network may be stated as follow:

$$\text{output} = f(W_2 \times (f(W_1 \times X + b_1)) + b_2) \quad (7)$$

where W_1 and W_2 indicate the layers of the weight matrix and b_1 and b_2 present the bias layers. Finally, the ANN formula for estimation of the compressive strength of mortars containing MK is presented as follows:

$$f_c = -\frac{48.2445}{1+e^{-\beta_1}} - \frac{21.7160}{1+e^{-\beta_2}} - \frac{227.2095}{1+e^{-\beta_3}} + 94.4652 \quad (8)$$

$$\beta_1 = 0.0042 \times (AS) - 0.0923 \times (MK\%) - 12.7028 \times (WB) + 196.7464 \times (BS) - 22.6704 \times (SP\%) - 59.7652$$

$$\beta_2 = -0.1010 \times (AS) + 0.0141 \times (MK\%) + 19.1848 \times (WB) - 60.6154 \times (BS) + 0.5999 \times (SP\%) + 22.3610$$

$$\beta_3 = -0.1646 \times (AS) + 0.0246 \times (MK\%) + 1.8258 \times (WB) - 31.9351 \times (BS) - 1.8524 \times (SP\%) + 8.1362$$

The performance statistics of the proposed formula are tabulated in Table 2. Accepted criteria introduced by Gandomi *et al.* [33] which recommended by Smith [34] for model validity. They expressed that if $|R| > 0.8$, an efficient correlation between the obtained and evaluated values existed. The evaluation measures presented in Table 2 confirm that the proposed formulae (Eq. 8) are capable of prediction of f_c in the mortars containing MK and gives a reasonable degree of accuracy.

Table 2

The criteria evaluations for f_c formula.

Method	Training			Validation			Testing		
	R	MSE	MAE	R	MSE	MAE	R	MSE	MAE
Proposed equation using ANN method	0.9865	4.6708	0.0622	0.9830	7.9386	0.1099	0.9754	10.0078	0.0808

Furthermore, a comparison between the measured and actual variables are depicted in Fig. 4. It is clear that as the ratios of actual to measured are close to one, the model yields proper accuracy. Therefore, according to Fig. 4 the distribution frequency of the actual to measured ratios presents remarkable accuracy of the proposed formulation.

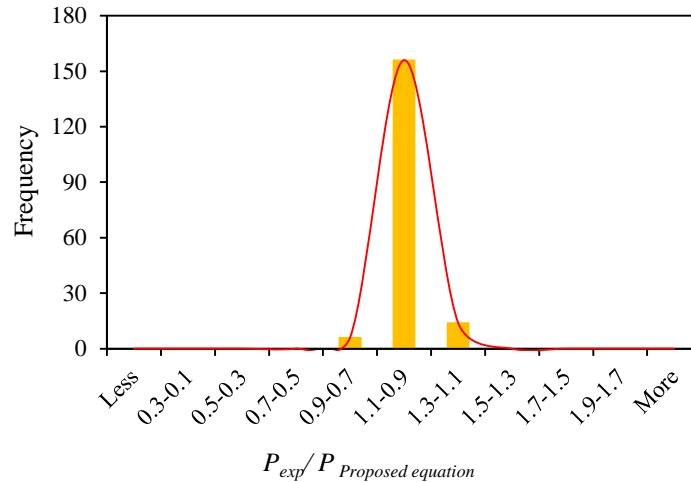


Fig. 4. The obtained results from developed formula vs. actual values.

4. Variables influences detection

An analysis is treated to predict the importance of input parameters relatively. Garson's algorithm [35] is employed to evaluate the relative importance of the inputs. Fig. 5 presents the sensitivity of input parameters. As shown in Fig. 5, *BS* exert dominant effects on the output. Therefore, based on the applied algorithm, the ratio of binder-sand probably exerts more effective influences on the f_c of mortars containing MK.

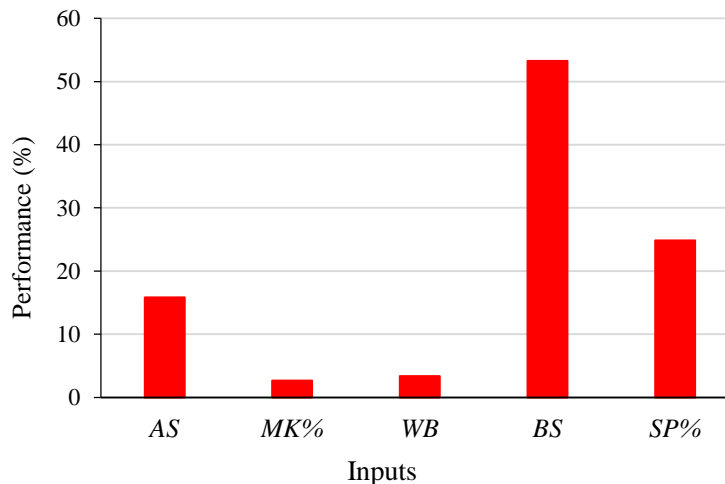


Fig. 5. Variables effectiveness of the ANN model.

Moreover, to picture confirmation of the developed ANN model, a parametric analysis has been also accomplished using a procedure introduced in Ref. [36]. The procedure examines the response of the developed formula to a set of assumed data. Based on this method, one input is changed while the other inputs remain constant at their average. If this analysis yields confirmed results to the underlying problem, the strength of the developed formula is proved. For this study, the results of the mentioned parametric analysis show in Fig. 6. Fig. 6 illustrates the tendency of the output predictions to the input variations. As expected, the f_c of mortars increase by

increasing of AS and also f_c of mortar decreased by increasing of WB ratio from 0.4 to 0.53. Therefore, these results confirm that the proposed formula is enough exact for use by practical engineers.

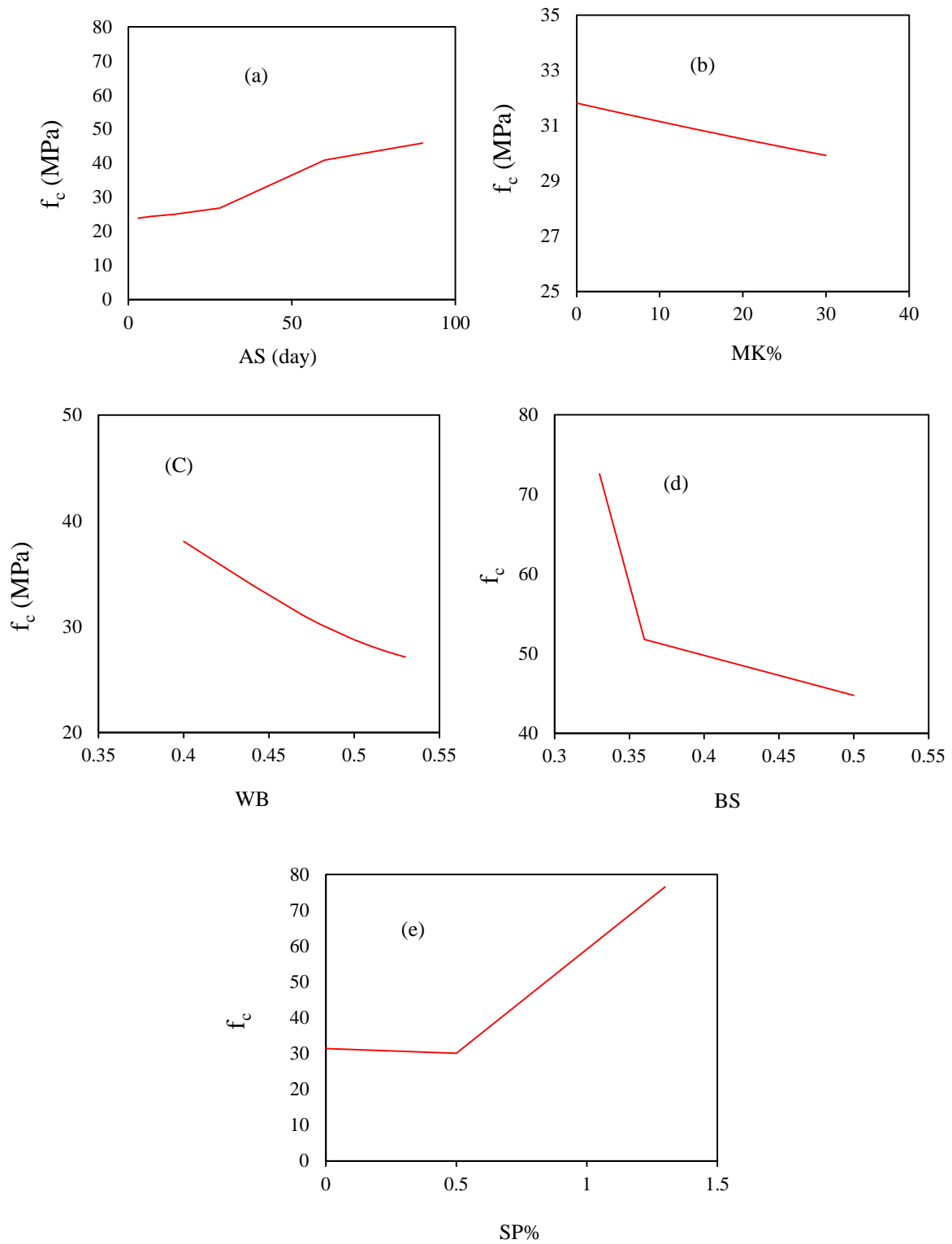


Fig. 6. Parametric analysis for f_c .

5. Conclusions

In the current article, the ANN was applied for the evaluation of the compressive strength of the mortars containing MK. The experimental dataset including 176 specimens was obtained using reliable literature for the ANN model development. Consequently, an ANN model consisting of three hidden layer neurons was constructed and five input parameters were considered including the age of the specimen, MK percentage, water-binder ratio, binder-sand ratio, and superplasticizer percentage. At the next, the new formulae based on the ANN were presented and performance analysis is undertaken for confirmation of this formula. The results showed that the new formulation based on the ANN, yielded a good accuracy by the r values of 0.9865, 0.9830 and 0.9754 for training, validating and testing datasets, respectively. Finally, the importance of each input parameter was determined by Garson's algorithm and it was found that the binder-sand ratio exerts more influence on the compressive strength of mortars containing MK than other effective factors. As a final point, the main objective of this study was developing a precise formulation for predicting the compressive strength of mortars containing MK. The new proposed formulae can be used by practical engineering applications.

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