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Modeling the compressive strength of cement mortar nano-composites

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Abstract. Nano-particle-reinforced cement mortars have been the basis of research in recent years and a significant growth is expected in the future. Therefore, optimization and quantification of the effect of processing parameters and mixture ingredients on the performance of cement mortars are quite important. In this work, the effects of nano-silica, water/binder ratio, sand/binder ratio and aging (curing) time on the compressive strength of cement mortars were modeled by means of artificial neural network (ANN). The developed model can be conveniently used as a rough estimate at the stage of mix design in order to produce high quality and economical cement mortars.

Keywords: cement mortar; nano particle; computer modeling; compressive strength; artificial neural networks; curing.

1. Introduction

Cement is a material which sets and hardens independently and can bind other materials together. It is commonly used as a basic ingredient of mortar and concrete. Mortar is a mixture of a binder material, water, and fine aggregate in the form of workable paste to bind construction blocks together and fill the gaps between them. A number of cementatious materials such as cement and lime may be used as binder constituent. However, cement mortar has special importance, because it is the basis for concrete (through the addition of aggregates).

Several parameters such as the properties of cement, presence of other cementitious and pozzolanic materials, incorporation of nano-sized particles in the binder mixture, water/binder ratio (water/cement ratio, if cement is the only binder material), amount of fine aggregate (sand), and mixing and curing conditions, are responsible for the performance and mechanical properties of cement mortar (Yeh 2008a, 2008b).

Nano-particles can be incorporated into conventional building materials to produce high performance ones. Mechanical properties of cement mortars with nano-SiO_2 and nano-Fe_2O_3 particles were studied before (Li *et al.* 2004a, 2004b). Experimental results demonstrated a significant change in compressive strengths of mortars that contained small amounts of nano-particles. Another study was carries out (Li *et al.* 2006) on cement mortars with nano-Al_2O_3. Other studies were generally concentrated on cement mortars with nano-SiO_2 (Jo *et al.* 2007, Qing *et al.* 2007, Lin *et al.* 2008).

Nano-particle reinforced cement mortars have been the basis of research in recent years and a

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significant growth is expected in the future. As a result, optimization and quantification of the effect of processing parameters and mixture ingredients on the performance of cement mortars are quite important (Peng *et al.* 2009). Unfortunately, accurate quantification and modeling of mortar and concrete mixtures and influence of processing parameters on their performance are still not available. This issue probably originates from the complexity of the system. The composition of the mortar (e.g. *wt*% of nano-SiO_2, water/binder ratio and sand/binder ratio), the size and shape of particles, the mixing method, and also several factors related to the aging practice (e.g. aging time and condition) are involved in this system. As a result, conventional modeling techniques are inappropriate to model this complex system. Therefore, powerful modeling techniques such as artificial neural network (ANN) can be helpful for this purpose (Oh *et al.* 1999, Kim *et al.* 2005, Yeh 2006, Gupta *et al.* 2006). ANN is based on available data and is commonly used to handle complex and nonlinear systems (Mirzadeh and Najafizadeh 2009a, 2009b, Hadi 2003). In recent years, artificial neural networks (ANNs) have been successfully applied to many engineering problems.

In this paper, the effects of nano-SiO_2 fraction in the binder mixture, water/binder ratio, amount of sand and aging time on the strengthening behavior of cement mortars were modeled and analyzed by means of ANN.

2. Methodology

2.1 Preprocessing

The database was taken from the literature (Li *et al.* 2004a, 2004b, 2006, Jo *et al.* 2007, Qing *et al.* 2007, Rao 2001). The nano-SiO_2 particles were added in the range of 0 to 10 weight percent to the binder mixture. The water/binder ratio and the sand/binder ratio were in the range of 0.3 to 0.65 and 0 to 3, respectively. The curing time was between 1 to 28 days and the values of compressive strength were in the range of 11 to 99 MPa. The representative histograms of available data are shown in Fig. 1(a).

The mixing practice employed in the cited references was as follows. The sand was added to the stirred mixture of cement, nano particles (if applicable) and water. The average diameter of nano-silica particles was between 15 to 40 *n*m. Therefore, one constituent of the resultant mortar mixer falls within the scope of nanomaterials (below 100 *n*m in three dimensions).

The 80 sets of available data were divided into three groups, 70% for the training set, 15% for the validation set and 15% for the test set. The validation set is used to control training process through the early stopping technique (Mirzadeh and Najafizadeh 2009a) and the testing set is used to evaluate the generalization ability of the trained network. The weight percent of nano-SiO_2 in the binder mixture, water/binder ratio, sand/binder ratio and aging time as input data were normalized in the range of -1 to 1 using Eq. (1) (Mirzadeh and Najafizadeh 2009b). The compressive strength values as output data were normalized in the range of 0 to 1 using Eq. (2) (Mirzadeh and Najafizadeh 2009b). It should be indicated that the binder mixture is composed of cement, pozzolanic materials and nano-particles.

$$x_n = 2\frac{x - x_{\min}}{x_{\max} - x_{\min}} - 1 \tag{1}$$

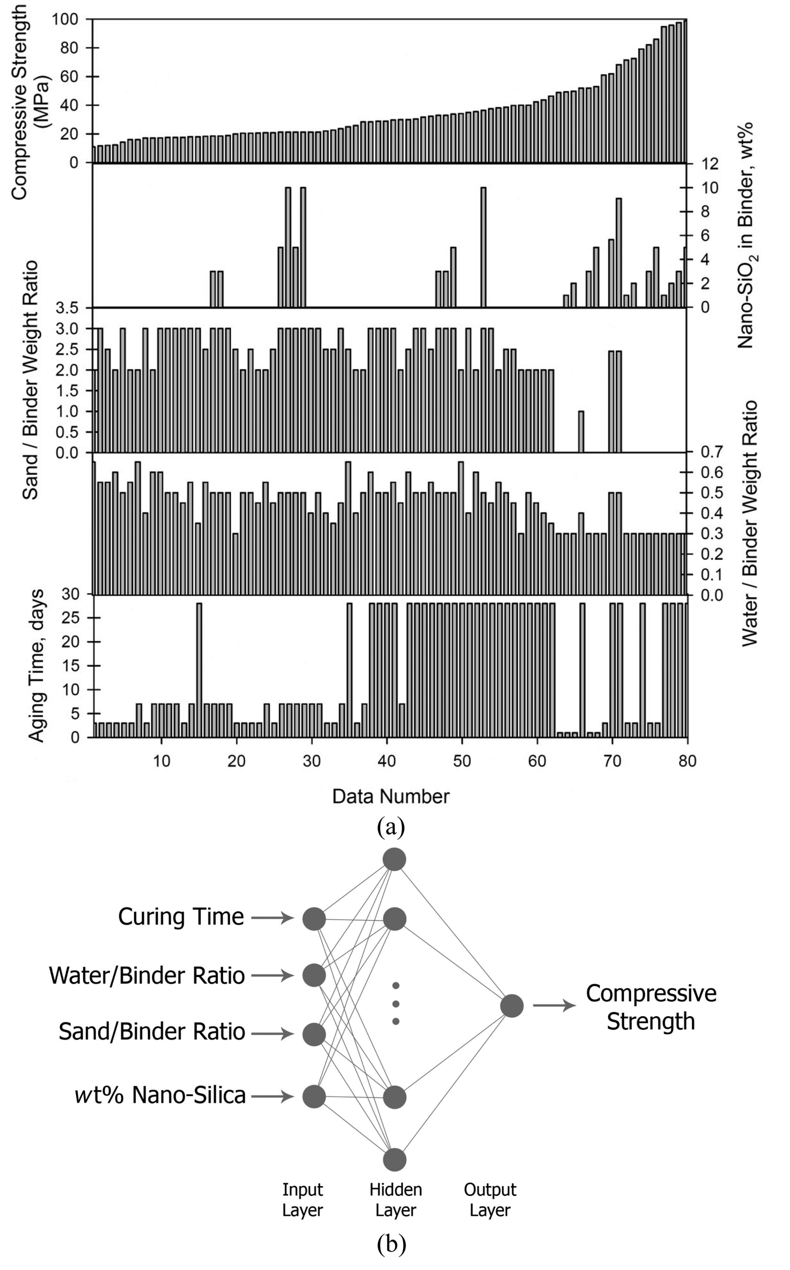


Fig. 1 (a) the representative histograms of available data and (b) schematic representation of the neural network architecture employed in this study

$$y_n = \frac{y - y_{\min}}{y_{\max} - y_{\min}} \tag{2}$$

Where, x_n and y_n are the normalized input and output values, respectively.

Among the affecting parameters mentioned above, the most important ones are aging time and mortar composition, which have been investigated repeatedly. However, very few systematic works are available on the effects of other parameters such as size and shape of particles and also the mixing method. As a result, the available literature is weak in this area. Therefore, these parameters were not considered in this work and some level of noise is inevitable. More experimental work could be helpful to overcome this problem.

2.2 Network design

A standard feed-forward network with one hidden layer was used in the present work and the optimal number of units in the hidden layer was determined by the trial and error procedure (Mirzadeh and Najafizadeh 2009a, 2009b). Fig. 1(b) shows a schematic representation of the neural network architecture employed in this study. The nonlinear logistic activation function (Mirzadeh and Najafizadeh 2009b) (Eq. (3)) was employed in the hidden layers.

$$y = \log sig(x) = \frac{1}{1+\exp(-x)} \tag{3}$$

2.3 Network training

The well-known back-propagation method is usually used to train ANNs. The early standard algorithm usually requires a lot of iterations to converge if it converges at all. Therefore, a number of variations of the standard algorithm have been developed. Among them, the Levenberg-Marquardt is the most popular one (Mirzadeh and Najafizadeh 2009a). This training algorithm was employed in this work using the neural network toolbox of MATLAB 7.4 in a dual-core processor based PC.

2.4 Stopping criterion

The neural network can be easily overtrained, in which the error rate on new unseen data becomes much larger than the error rate on the training data. Therefore, it is important not to overtrain the network. A good method for choosing the number of training epochs (iterations) is the early stopping technique (Mirzadeh and Najafizadeh 2009a). In this technique, the training process must be stopped when the error measured using an independent validation set starts to increase. This method was used in the present work.

2.5 Network testing

If the network is properly trained, it has then learned to model the function that relates the input variables to the output variables and can subsequently be used to make predictions where the output is not known. This ability is called generalization (Mirzadeh and Najafizadeh 2009b). In this paper the test set was used to evaluate the generalization ability of the trained network.

The generalization ability of the model was determined by drawing a scatter diagram of predicted values versus measured values and calculating the root mean square error by using the equation below (Mirzadeh and Najafizadeh 2009a)

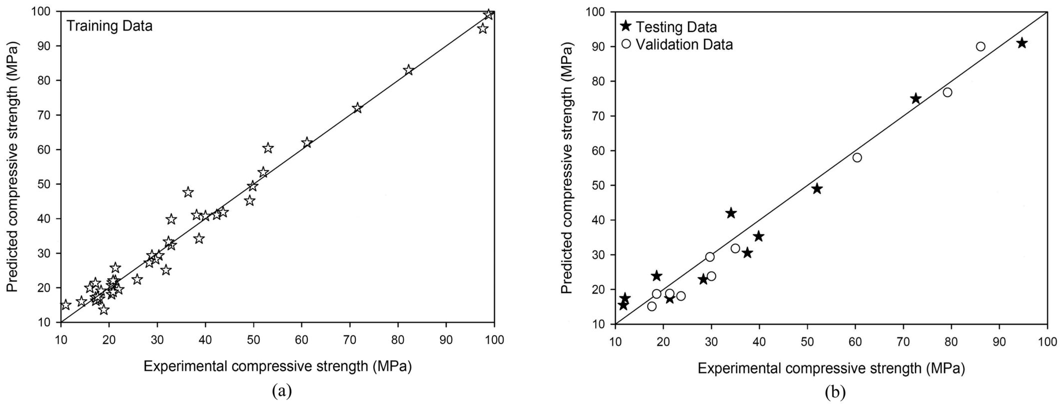


Fig. 2 Scattered diagram of predicted values versus measured values: (a) training data and (b) testing and validation data

$$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(t_i - y_i)^2} \tag{4}$$

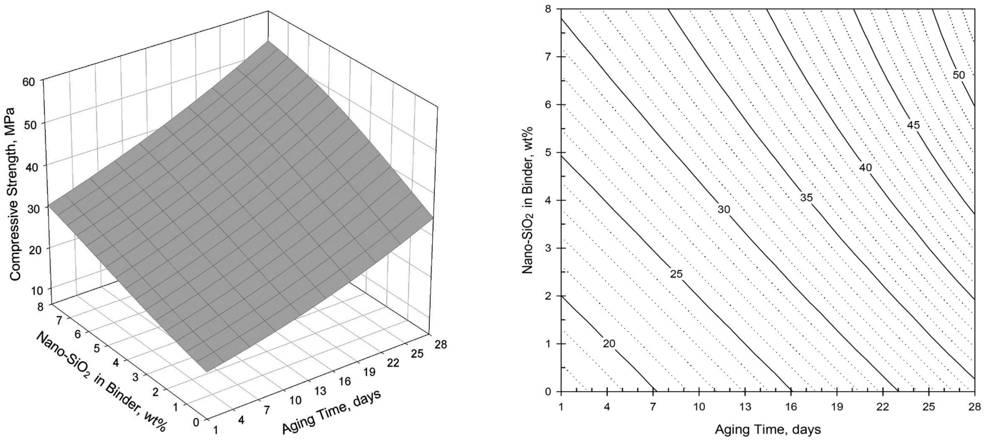
The scatter diagram of predicted values versus measured values for training, testing and validation data is shown in Fig. 2. It shows that the model prediction fits well with the experimental observations. The developed network shows good performance and network results are in a good agreement with experimental data taken from literature. The RMSE for the training and the test sets was respectively determined as 2.24 and 4.73 MPa, which confirms the applicability of this ANN model for prediction of compressive strength of cement mortars.

It should be indicated that the emphasis of this paper is on the applications of ANN as a powerful modeling technique in the field of building materials science and technology. Therefore, the method used was briefly explained here and more details can be found elsewhere (Mirzadeh and Najafizadeh 2009a, 2009b).

3. Results and discussion

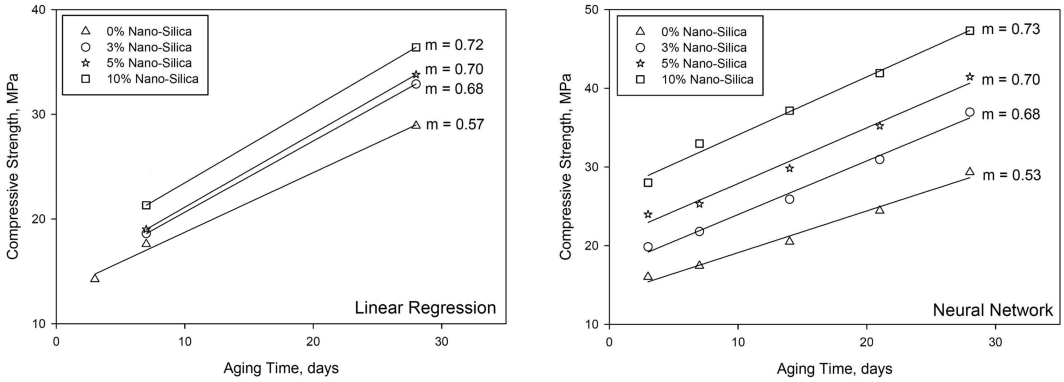
3.1 Effect of aging time and nano-silica

Fig. 3(a) shows the response surface of compressive strength as a function of aging time and weight percent of nano-SiO_2 by using the results of ANN model. The strength increases by aging time and also by increasing the nano-SiO_2 content in binder. Experimental results (Li *et al.* 2004a) demonstrated an increase in compressive strength of mortars containing nano-particles. Scanning electron microscopy (SEM) proved that the nano-SiO_2 particles fill the pores and also reduce the content of $Ca(OH)_2$ within the hydration products. Moreover, the nano-particles are uniformly dispersed in the cement paste, the hydrate products of cement will deposit on the nano-particles due to their great surface energy during hydration and grow to form conglomerations containing the nano-particles as ‘nucleus’. The nano-particles located in the cement paste as nuclei will further promote and accelerate cement hydration due to their high effective surface. These effects are responsible for the improvement of compressive strength of mortars with nano-particles. Experimental



(a) (b)

Fig. 3 (a) response surfaces and (b) contour lines of compressive strength as a function of aging time and weight percent of nano-SiO_2 at sand/binder ratio of 2.5 and water/binder ratio of 0.5



(a) (b)

Fig. 4 Investigating the effect of aging time and weight percent of nano-SiO_2 at sand/binder ratio of 3 and water/binder ratio of 0.5 using: (a) linear regression analysis and (b) neural network results

observations show that the use of nano-SiO_2 leads to increase of both early age and ultimate strength of cement mortar (Li *et al.* 2004a). This is consistent with the results presented in Fig. 3(b). This figure shows the contour lines of compressive strength as a function of aging time and weight percent of nano-SiO_2. By using this figure, the compressive strength of cement mortars with different amounts of nano-SiO_2 can be taken at any stage of curing.

As stated before, the relationships are non-linear and neural network is a promising method for this modeling work. By the way, the required data set for comprehensive linear regression analysis is not available. However, linear regression can be applied to available data to deduce some interesting points. Fig. 4(a) shows the effects of aging time and weight percent of nano-SiO_2 on the compressive strength using the linear regression method. It can be seen that by increasing the amount of nano-SiO_2 in the binder mixture, the slope of the regression lines increases and thereby the effect of aging time becomes more pronounced. Fig. 4(b) shows similar figure drawn using the results of neural network. Both figures show similar slope for a given amount of nano-SiO_2.

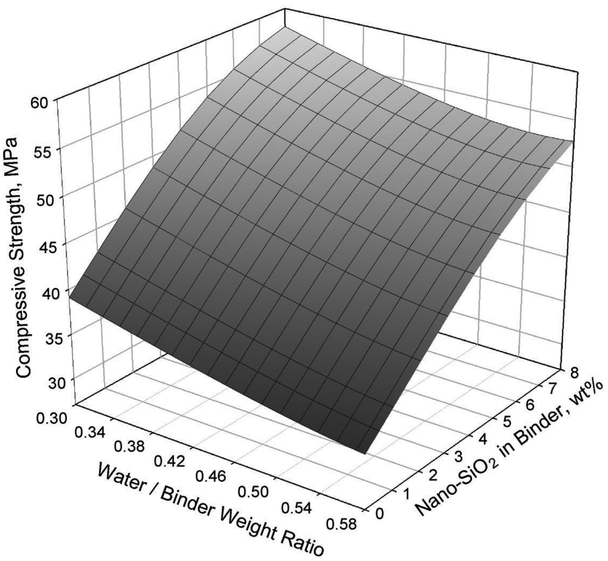


Fig. 5 Response surface of compressive strength at 28th day as a function of water/binder ratio and weight percent of nano-SiO_2 with sand/binder ratio of 2.5

3.2 Effect of water/binder ratio and nano-silica

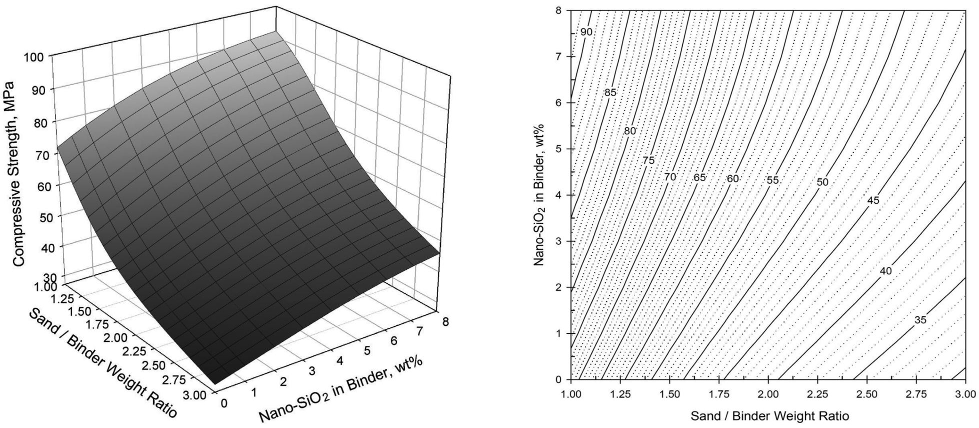
Fig. 5 depicts the response surface of compressive strength as a function of water/binder ratio and weight percent of nano-SiO_2. The strength increases by increasing nano-SiO_2 content in binder and decreasing water/binder ratio.

If the water/binder ratio is held below a certain value at mixing, the strength of concrete and cement mortars are assumed to be of acceptable standards at later ages. Generally, the strength is characterized by the result of compressive tests at 28 days curing time. However, quality evaluation at earlier ages, even fresh concrete and cement mortar, is highly desirable (Philippidis and Aggelis 2003). The increase in strength with aging time can be attributed to the time dependency of cement hydration process. The water is responsible for early strength development. Therefore, a very low water/binder ratio will be detrimental to the strength. However, increasing the water/binder ratio increases the porosity content that results in decrease in the strength and increase in the permeability (Bescher *et al.* 2004). Moreover, excessive water will lead to increased bleeding (appearance of surface water) and also segregation of sand particles, which result in the reduction of mortar quality.

The figure also indicates that adding nano-SiO_2 in binder is more effective than changing the water/binder ratio. Therefore, by addition of nano-SiO_2, higher water/binder ratios can be used in order to improve the workability of the mortar mixture, while maintaining the desired compressive strength. However, in practice, due to high water absorption of these small particles, the majority of mixing water is normally consumed by nano particles. Therefore, the application of high amount of nano-SiO_2 may not be possible at very low water/binder ratios.

3.3 Effect of sand/binder ratio and nano-silica

Fig. 6(a) shows the response surface of compressive strength as a function of sand/binder ratio



(a) (b)

Fig. 6 (a) response surface and (b) contour lines of compressive strength at 28th day as a function of sand/binder ratio and weight percent of nano-SiO_2 in binder with water/binder ratio of 0.5

and weight percent of nano-SiO_2. The strength decreases by increasing sand/binder ratio. This effect can be easily explained by the fact that a higher sand/binder ratio is equivalent to lower binder content in the mortar mixture. However, mortars with high cement content are undesirable due to economical considerations.

The figure also shows that sand/binder ratio has a significant effect on the compressive strength. The total surface area of sand particles (fine aggregates) in cement mortar is very high. Therefore, the compressive strength of cement mortar is highly sensitive to sand/binder ratio, which its surface area is higher than the total surface area of concrete aggregates that composed of fine and coarse aggregates.

Therefore, the strength of cement mortar can be adjusted by addition of nano-SiO_2 in binder mixture and variation of sand/binder ratio. This effect is shown in Fig. 6(b) by contour lines of compressive strength as a function of sand/binder ratio and weight percent of nano-SiO_2 in binder.

4. Conclusions

The effects of nano-SiO_2 addition, water/binder ratio, sand/binder ratio and aging (curing) time on the compressive strength of cement mortars were modeled and analyzed by means of artificial neural network (ANN). The results of the ANN model were in a good agreement with the experimental data taken from the literature. The appropriate range of processing parameters for enhancing the compressive strength of cement mortars can be determined from the resultant figures generated by neural network. These results can be conveniently used as a rough estimate at the stage of mix design in order to produce high quality and economical cement mortars. This goal can be achieved by introducing small amount of nano-SiO_2 in the binder mixture based on the predictions of ANN, and considering suitable values for the sand/binder and water/binder ratios.

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