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The use of artificial neural networks in predicting ASR of concrete containing nano-silica

Ramin Tabatabaei*, Hamid Reza Sanjari[a] and Mohsen Shamsadini[b]

Department of Civil Engineering, Islamic Azad University, Kerman Branch, Kerman, Iran

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Abstract. In this article, by using experimental studies and artificial neural network has been tried to investigate the use of nano-silica as concrete admixture to reduce alkali-silica reaction. If there are reactive aggregates and alkali of cement with enough moisture in concrete, a gel will be formed. Then with high reactivity between alkali of cement and existence of silica in aggregates, this gel will expand by absorption of water, and causes expansive pressure and cracks be formed. At the time passes, this gel will reduce both durability and strength of the concrete. By reducing the size of silicate to nano, specific surface area of particles and number of atoms on the surface will be increased, which causes more pozzolanic activity of them. Nano-silica can react with calcium hydroxide (Ca $(OH)_2$) and produces C-S-H gel. In this study, accelerated mortar bar specimens according to ASTM C 1260 and ASTM C 1567, with different mix proportions were prepared using aggregates of Kerman, such as: none admixture and plasticizer, different proportions of nano-silica separately. By opening the moulds after 24 hour and curing in water at 80 ℃ for 24 hour, then curing in (1N NaOH) at 80 ℃ for 14 days, length expansion of mortar bars were measured and compared. It was noted that, the lowest length expansion of a specimens shows the best proportion of admixture based on alkali-silica reactivity. Then, prediction of alkali-silica reaction of concrete has been investigated by using artificial neural network. In this study the backpropagation network has been used and compared with different algorithms to train network. Finally, the best amount of nano silica for adding to mix proportion, also the best algorithm and number of neurons in hidden layer of artificial neural network have been offered.

Keywords: Nano-Silica; Alkali-Silica Reaction (ASR); Mix Design; Artificial Neural Network (ANN), Backpropagation

1. Introduction

Nowadays, with increase of using concrete and emergence of Nano technology, it is necessary to study various properties of concrete containing nano-particles and their effects on the improvement of concrete properties. The properties of concrete can be studied based on workability, strength and durability. One of the factors that affect the durability of concrete is alkali-silica reaction (ASR).

*Corresponding author, Assistant Professor, E-mail: tabatabaei@iauk.ac.ir
[a]Researcher, E-mail: hsanjary@yahoo.com
[b]Researcher

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As shown in Fig. 1, if reactive aggregate and alkali of cement with enough moisture in concrete exist, a gel will be formed in concrete and with increase of reactivity of alkali in cement and existence of silica in aggregates, this gel absorbs water and causes expansion pressure and cracks be formed. At the time passes, this gel will reduce both durability and strength of the concrete (Kosmatka *et al*. 2003). This reaction is called alkali-silica reaction or cancer of concrete. Three conditions are necessary for alkali-silica reaction to take place, these condition are: active forms of silica in aggregates, highly alkaline pore solution and enough moisture (Lukschová *et al*. 2009). The cracks due to ASR have been shown in Fig. 2.

By reducing the size of silicate to nano, specific surface area of particles and number of atoms on the surface will be increased which causes more pozzolanic activity of them. Nano-silica will react with calcium hydroxide ($Ca\ (OH)_2$) and will produce C-S-H gel. By using nano-particles and reducing crystal size and amount of calcium hydroxide, C-S-H gel fills the void spaces of interfaces of the typical aggregates and cement and make it denser. Nano particles can fill empty spaces of C-S-H gel as well and make it denser (Ramazanianpour *et al*. 2009).

Previous researches involving the use of various materials such as: fly ash, pozzolan, rice husk, micro-silica (silica fume), nano-silica, as admixture in concrete in order to increase the strength and durability of concrete with specific proportion of mixtures. See (Qurecaia and Brouwers 2010) and (Alavi and Mirzadeh 2012). Admixtures such as fly ash, slag, silica fume and natural pozzolans like calcinations of clay and schist to improve the specific properties of concrete such as mitigation of alkali-silica reaction is used (Kosmatka *et al*. 2003 and Al-Chaar *et al*. 2013). Previous studies show that, the use of silica fume and nano silica with certain proportion increases the compressive strength of concrete in comparison with specimens. In the same proportion, nano silica gained higher compressive strength and lower water abortion to silica fume (Ramazanianpour *et al*. 2009). The use of nano silica in concrete containing natural pozzolan reduces strength in its early life, but significantly increases compressive and flexural strength of concrete (Maghsoudi and Ahmadi Mogadam 2007). The artificial neural network in predicting the compressive strength and abrasion of concrete, roller concrete mix design and other concrete properties has been used. See (Boukhatem *et al*. 2012), (Ramazanianpour and Rahmani 2006) and (Ramazanianpour and Sadeghi 2006).

An analytical model artificial neural networks (ANN) as a substitute in simulation is used to simulate the corrosion induced crack width. However when dealing with random fields, the Monte Carlo simulation is apparently an inefficient and time consuming method, hence the previous studies are shown the ANN is found very capable (Firouzi and Rahai 2013).

The aim of this study is to investigate the effect of nano silica on alkali-silica reaction of concrete and has been tried by using results of tests and artificial neural network to predict the expansion of specimens.

It has been tried to model the results of experiments by using backpropagation artificial neural network in MATLAB to predict alkali-silica reactivity of concrete containing nano silica. In this network, input vectors and the corresponding target vectors have been used to train the network until it can approximate a function, associate input vectors with specific output vectors, or classify input vectors in an appropriate way as defined by designer.

Backpropagation was created by generalizing the Widrow-Hoff learning rule to multiple layer networks and nonlinear differentiable transfer functions. Input vectors and the corresponding target vectors are used to train a network until it can approximate a function, associate input vectors with specific output vectors, or classify input vectors in an appropriate way as defined by user. Standard backpropagation is a gradient descent algorithm, in which the network weights are moved along

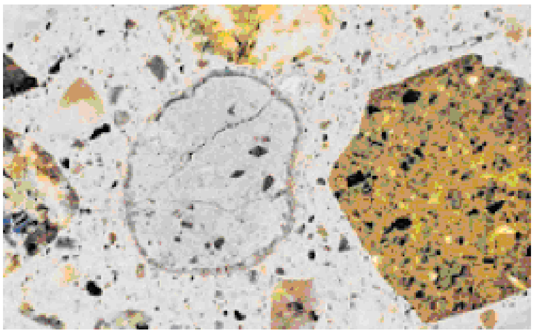

Fig. 1 Polished section view of an alkali reactive aggregate in concrete. Observe the alkali silica reaction rim around the reactive aggregate and the crack formation, (Kosmatka *et al*. 2003)

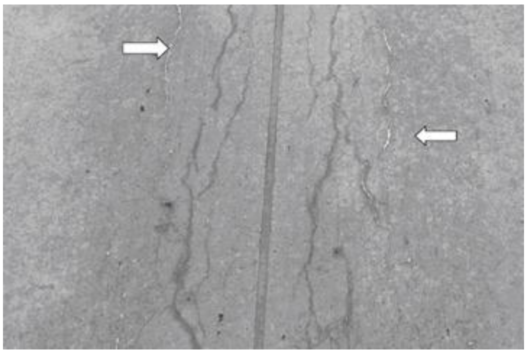

Fig. 2 Cracking with white ASR exudates (arrows) in cracks, (Van Dam and Peshkin 2009)

the negative of the gradient of the performance function. The term backpropagation refers to the manner in which the gradient is computed nonlinear multilayer networks (Beale *et al*. 2010).

The Levenberg-Marquardt algorithm was designed to approach second order training speed without having to compute the Hessian matrix. When the performance function has the form of a sum of squares, then the Hessian matrix can be approximated as Eq. (1) and the gradient can be computed as Eq. (2), where J is the Jacobian matrix that contains first derivatives of the network errors with respect to the weights and biases, and e is a vector of network errors. The Jacobian matrix can be computed thought a standard backpropagation technique that is much less complex than computing the Hessian matrix (Beale *et al*. 2010).

$$H = J^T J \tag{1}$$

$$g = J^T e \tag{2}$$

The Levenberg-Marquardt algorithm uses this approximation to the Hessian matrix in the following in the following Newton like update Eq. (3),

$$X_{k+1} = X_k - [J^T J + \mu I]^{-1} J^T e \tag{3}$$

When the scalar μ is zero, this is just Newton's method, using the approximate Hessian matrix. When μ is large, this becomes gradient descent with a small step size. Newton's method is faster and more accurate near an error minimum, so the aim is to shift towards Newton's method as quickly as possible. Thus, μ is decreased after each successful step (reduction in performance function) and is increased only when a tentative step would increase the performance function. In this way, the performance function will always be reduced at each iteration of the algorithm (Beale *et al*. 2010).

In the present work, different algorithms and different number of neurons in hidden layer has been used to train the backpropagation network in this study and results have been compared.

2. Experimental

2.1 Materials

The brand of used nano-silica is AEROSIL 200 degussa, average primary particle size is 12 nm, the specific surface area is 200±25 m^2/g, SiO_2 content ≥ 99.8 wt. %, pH of particle is between 3.7-4.7, moisture is ≤ 1.5 wt. %. The used micro-silica has been produced in Iran ferroalloy industries, in Azna city, the specific surface area is 20-25 m^2/g. The cement has been used from Portland cement type 1-425. The aggregates have been used from the mines of around the city of Kerman. The water of mixture has been used from water of Kerman. The used NaOH has been produced in Iran.

2.2 Mix proportion

In this study the method of accelerated mortar bar has been used to evaluate alkali-silica reaction. For this purpose 6 mix proportions are used as follow: one of the mix designs was without any admixture and used for testifier and the other 5 mix designs were prepared by adding different proportion of nano silica to mix design. Mix proportions have been prepared based on the standard of accelerated mortar bars. See ASTM C 1260 (1994) and ISIR 8753 (1993). In order to precisely evaluate the effect of admixtures in mortar mix proportions, use of plasticizer were avoided and water-cement ratio around 0.47 were used for all mix proportions. Details of mix proportion, their names and the quantity of materials for preparation of 3 specimens for each mix proportion have been mentioned in Table 1. The amount of nano silica that has been listed in Table 1 is based on the percentage mass of cement.

Table 1 Mix proportions

Proportion name	Cement gr	Aggregate gr	w/c	Micro silica gr	Nano silica gr
OC	440	990	0.47	0	0
N5	440	990	0.47	0	5%
N10	440	990	0.47	0	10%
N20	440	990	0.47	0	20%
N30	440	990	0.47	0	30%
N40	440	990	0.47	0	40%

2.3 Preparation and maintenance of specimens

In order to test accelerated mortar bar, ASTM C 1260, ASTM C 1567, three specimens in metal molds for each plan were prepared. Used aggregates must meet the aggregation requirements of experiments. After molding and preparing the mix proportion, specimens should be covered and cured in chamber with plastic bags within 24 hours. After removing them from molds, specimens should be cured in water for 24 hour at 80^{o}C, then in 1N NaOH for 14 days at 80^{o}C. To make 1 liter solution of 1N NaOH, 40 gr sodium hydroxide was dissolved in 900 ml water and then diluted with water to reach the volume of 1 liter. Expansions of specimens were measured after 1, 7 and 14 days curing in the solution. If the average expansion of control specimens after curing in solution is less than 0.1%, the aggregates represents the inactivity of aggregates and if the expansion is between 0.1% and 0.2% represents the potential of destructive reactivity and if the expansion of specimens is more than 0.2% represents destructive reactivity of aggregates See ASTM C 1260 (1994) and ASTM C 1567 (2004).

2.4 Model of artificial neural network

Different learning algorithms can be used in backpropagation network. In this model, different algorithms have been used to train the network such as: Scaled Conjugate Gradient, BFGS, One Step Secant and Levenberg-Marquardt. Also, the effect of number of neurons in hidden layer of each algorithm on the epochs and error rate of each algorithm has been investigated.

If linear output neurons are used the network outputs can take any value. In this model, the backpropagation network with Tan-sigmoid (hyperbolic tangent sigmoid) transfer function in one hidden layer and linear transfer function (pure line) in output layer has been used. The Fig. 3 shows the used model of network and Fig. 4 shows the transfers function of used network.

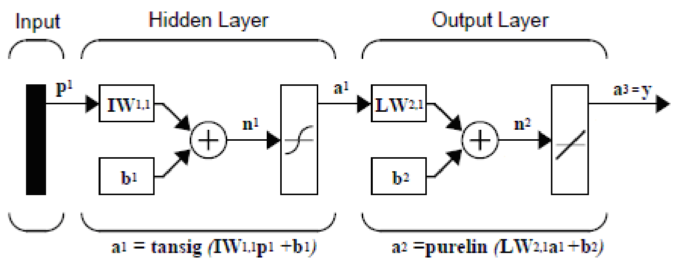

Fig. 3 The model of network with Tan-Sigmoid transfer function in hidden layer and linear transfer function in output layer (Beale *et al*. 2010)

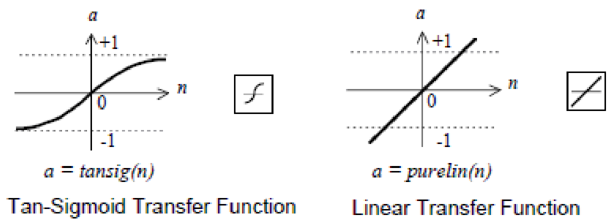

Fig. 4 The Tan-Sigmoid and linear transfer function (Beale *et al*. 2010)

3. Results and discussion

In the present work, alkali-silica reaction (ASR) potential of aggregates has been investigated in experimental real concrete specimens including nano silica.

Usually, the extent of ASR will depend on factors such as the nature and reactivity level of the aggregate; however, the rate of expansion has been reduced compared to higher humidity conditions.

The addition of nano silica enhances the possibility for the reaction with calcium hydroxide (CH) to develop more strength carrying structure of cement in the shape of calcium silica hydrate (C-S-H) and also micropore-filling consequence of nano silica in the hardened concrete. Chemically, using the well dispersed nano silica act as crystallization centres of the hydrated products, in that way increasing the hydration rate, that is, nano silica assisted towards the formation of smaller size CH crystals and homogeneous clusters of C-S-H composition. Moreover, the nano silica improved the structure of the transition zone between aggregates and paste, (Maheswaran *et al*. 2013).

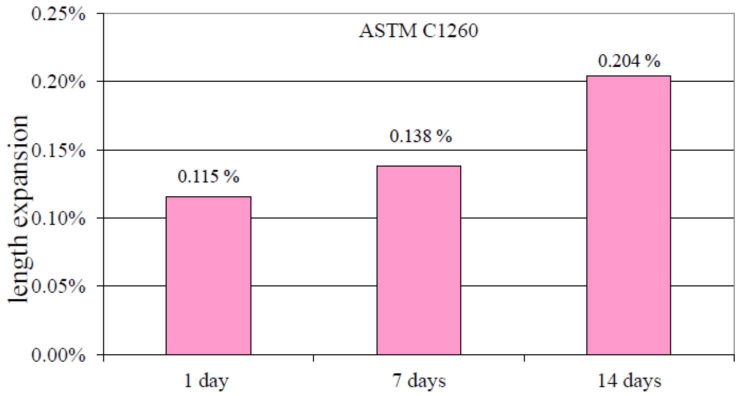

Fig. 5 Result of accelerated mortar bar experiments (control specimens)

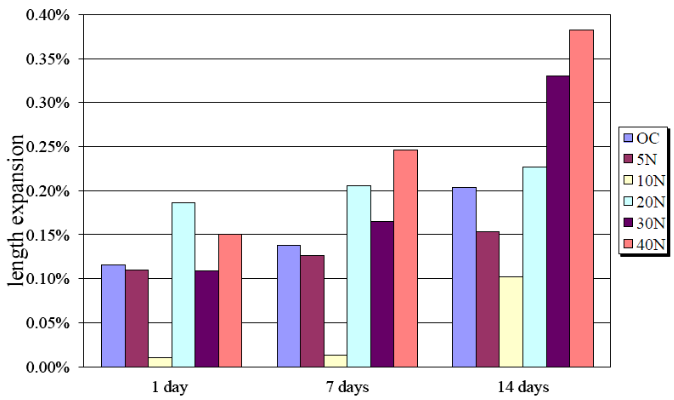

Fig. 6 Comparison of experimental results

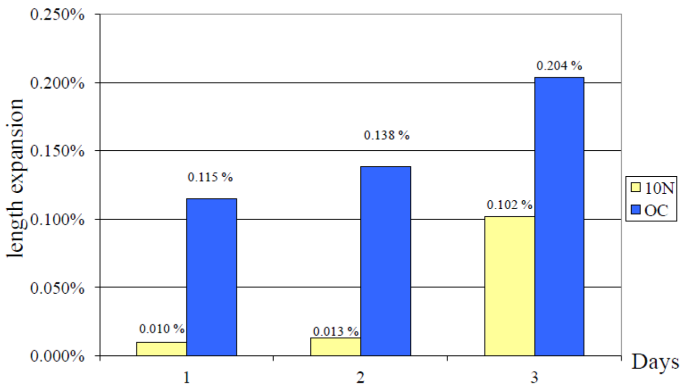

Fig. 7 Comparison of the results of adding 10% mass of cement with nano silica and control specimens

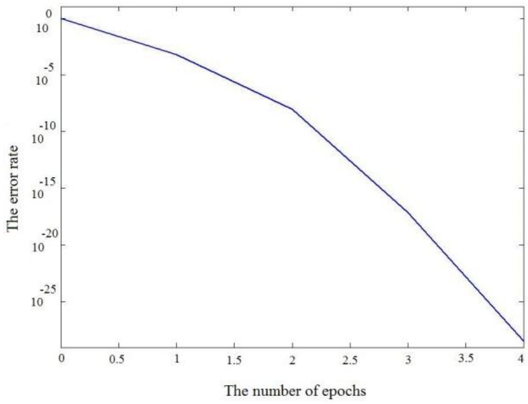

Fig. 8 The relation between number of epochs and rate of errors in Levenberg-Marquardt algorithm with 24 neurons in hidden layer

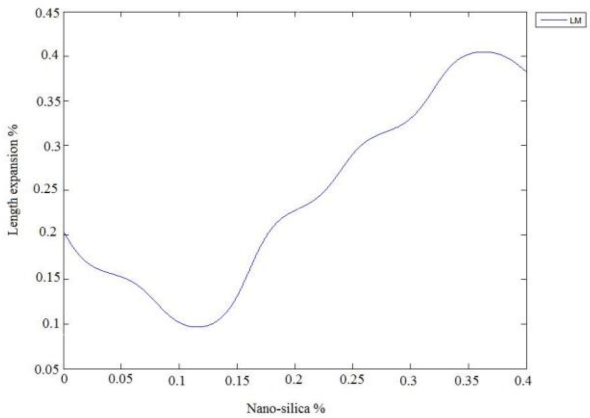

Fig. 9 The relation between amount of nano-silica in mixture and length expansion of specimens after 14 days curing in (1N NaOH) at 80^{o}C

Table 2 Comparison of the number of neurons in hidden layer and the epoch of training the network by different algorithms

Number of epochs in different algorithms				
Levenberg marquardt	One step secant	BFGS	Scaled conjugate gradient	Number of neurons in hidden layer
5	65	18	14	6
3	46	11	16	12
3	68	10	15	18
4	40	10	16	24
4	47	9	15	100

Table 3 Comparison of the number of neurons in hidden layer and the error of training network by different algorithms

Number of epochs in different algorithms				
Levenberg marquardt	One step secant	BFGS	Scaled conjugate gradient	Number of neurons in hidden layer
$7e^{-14}$	$8e^{-7}$	$9e^{-8}$	$2e^{-5}$	6
$3e^{-11}$	$3e^{-8}$	$7e^{-7}$	$5e^{-5}$	12
$1e^{-10}$	$2e^{-7}$	$2e^{-7}$	$6e^{-5}$	18
$4e^{-11}$	$3e^{-6}$	$1e^{-7}$	$7e^{-5}$	24
$1e^{-11}$	$2e^{-6}$	$1e^{-9}$	$4e^{-5}$	100

The potential for further expansion due to ASR is one of the most important parameter in the process of assessing the current condition of ASR effect of the specimens. The monitoring of the current deformations is the only accurate method of estimating ASR potential. After measuring the expansion of the control specimens according to ASTM C 1260, Fig. 5 represents the used aggregates which have the potential of reactivity.

The average of three specimens with six different percentages of nano silica categories was used to get the final expansion result of the testing procedures. Fig. 6 shows the test results of specimens compared with each other and with control specimens according to ASTM C 1260 and ASTM C 1567.

Mixture proportions used for these tests are listed in Table 1 that includes mixture properties including % nano silica. In this study, expansion data were recorded after zero-day of curing and then every 1, 7 and 14 days. The average mortar expansions of more than 20% nano silica show that all percentages of this have not improved the ASR effect. This matter is illustrated in Fig. 6.

According to the result of Fig. 6, the best results were obtained by adding nano silica with amount of 10% mass of cement. In Fig. 7, this proportion has been compared with control specimens.

In Table 2, the effect of the number of neurons in hidden layer has not been affected so much on the error of network in investigated algorithms have been mentioned. By comparing of these results, the minimum epoch of network has been obtained from Levenberg-Marquardt algorithm and high increase of the number of neurons in hidden layer have not been affected so much on the epochs of these algorithms.

In Table 3, the effect of number of neurons in hidden layer on the error rate of algorithms of the

backpropagation artificial neural network has been mentioned. By comparing these results, the minimum epoch of network has been obtained from Levenberg-Marquardt algorithm and high increase of the number of neurons in hidden layer has not been affected
so much on the error of network in investigated algorithms.

The relation between error rate and number of epoch in artificial neural network which has been obtained from Levenberg-Marquardt algorithm whit 24 neurons in hidden layer has been showed in Fig. 8.

The relation between percentage of nano silica in mixture and length expansion of specimens after 14 days curing in (1N NaOH) at 80^{o}C which have been obtained from Levenberg-Marquardt algorithm (LM) in artificial neural network has been showed in Fig. 9.

4. Conclusions

1) Addition of 5% and 10% mass of cement with nano silica to mix proportions caused the reduction of expansion of mortar bars.

2) By adding more than 10% mass of cement with nano silica, good results were not obtained and even more expansion of specimens in comparison with control specimens were observed.

3) Comparing the result of adding 5% and 10% mass of cement with nano silica shows that 10% nano silica reduced more expansion of accelerated mortar bars.

4) Comparison between use of the Levenberg-Marquardt algorithm and the other investigated algorithms to train the backpropagation artificial neural network shows that the Levenberg-Marquardt algorithm has been obtained fewer epochs and less error in the network.

5) In this backpropagation artificial neural network, consuming the number of neurons in hidden layer with equal or twofold of inputs to train the network in different various algorithms were obtained better results.

The results of this study are limited to the used materials, experimental conditions and the consumed algorithms and network. Additional experiments like petrography tests such as XRD, SEM, TEM and also studies of the other properties of concrete and artificial neural network are needed.

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