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THE USE OF ARTIFICIAL NEURAL NETWORK TO PREDICT COMPRESSIVE STRENGTH OF GEOPOLYMERS

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ABSTRACT

In order to predict compressive strength of geopolymers based on the effect of Al_2O_3/ SiO_2, Na_2O/Al_2O_3, Na_2O/H_2O, and Na/[Na+K], more than fifty data were gathered from the literature. These data were utilized to train and test the three layer artificial neural network. In this study, feed forward networks with various numbers of hidden layers and neurons are tested to select the optimum network architecture. The developed neural network simulator model has used the feed-forward back propagation architecture and this demonstrates its ability in training the given input/output patterns. A multi-layer feed forward network is designed with chemical compositions of alumina silicate and alkali activators as inputs and compressive strength as output. This leads to the optimum chemical composition and the best paste can be made from activated alumina silicate waste materials using alkaline hydroxide, and alkaline silicate. The neural network models give high prediction accuracy and the research results conform to some rules of geopolymer binders chemical compositions.

Keywords: artificial neural network, geopolymers, feed forward network, back propagation, and activated alumina silicate waste

INTRODUCTION

The reaction of reactive alumina silicates such as natural pozzolan, metakaolin and pozzolanic by products like slags and flyash with highly concentrated alkali hydroxide or silicate solution produces a kind of amorphous alumina silicate which was first discovered by Chelokovski in 1950 and then called geopolymer by Devidovits (Devidovits, 1991). This material exhibits good properties such as designable setting time, moderate to high compressive strength, low shrinkage and high sulphate resistance with low environmental impacts which makes it a good candidate to be replaced to ordinary Portland cement in order to reduce greenhouse emissions comparable to traditional cement (Devidovits, 1994).

Geopolymer properties should be optimized in accordance with the application and the properties which are expected of them. One of the geopolymer materials applications is to be consumed as a replacement of Portland cement which causes to categorize them with different specifications and mechanical properties. These properties are depended to the combined effects of Al_2O_3/SiO_2, Na_2O/Al_2O_3, Na_2O/H_2O, and Na/[Na+K] molar ratios in the alumina silicate and alkali activators compositions (Barbosa et al., 2000 and Duxson, 2005).

Recently some of the researchers have used ANN for the prediction of mechanical properties of construction materials such as concrete and it is expected that the number of experiments to investigate the effect of chief parameters on mechanical properties can be reduced (Lai & Sera, 1997, Mandal & Roy, 2006, Sebastia et al., 2003, and Topcu & Saridemir, 2008).
For optimization the first step involves designing the network and then the selection of initial weights and biases and finally using the best algorithm to change weights and biases during the learning process to find the best weight and biases in order to produce the desirable outputs from the input pattern (Topalov & Kaynak, 2004 and Topcu & Saridemir, 2008). Most researchers prefer feed forward ANN and use the back propagation method for training (Mandal & Roy, 2006). In this method, in every interval, output is computed from the input pattern with current weights and biases and in the second step weights and biases are changed with a backward algorithm. The performance functions (usually mean square error or sum square error) are minimized by changing the weights and biases step to step.
Generalization of the network and selection of learning algorithm are based on the input data. Every selected algorithm has some advantages and disadvantages. Thus choosing a suitable algorithm usually has no special discipline and comes with experience. One of the best training algorithms, having a fast rate of convergence is traingda. Traingda can train any network as long as its weight, net input, and transfer functions have derivative functions. Back propagation is used to calculate derivatives of performance dperf with respect to the weight and bias variables X. Each variable is adjusted according to gradient descent:

$$*dX = lr*dperf/dX \tag{1}$$

At each epoch, if performance decreases toward the goal, then the learning rate is increased by the factor lr_inc. If performance increases by more than the factor max_perf_inc, the learning rate is adjusted by the factor lr_dec and the change that increased the performance is not made (Koker et al., 2005).
One of the problems that occur during ANN training is called over fitting. The error on the training set is driven to a very small value, but when new data is presented to the network the error is high. The network has memorized the training examples, but it has not learned to generalize the new situations. The best way to avoid over fitting is to use lots of training data (Mandal & Roy, 2006 and Yang et al., 2004). Although this is impossible in some case due to increasing time and cost of experiments. Thus most important methods for improving network generalization and avoid over fitting are model selection, early stopping, weight decay and combining networks. In traingda algorithms training stops when any of these conditions occurs:

* The maximum number of epochs (repetitions) is reached.
* The maximum amount of time is exceeded.
* Performance is minimized to the goal.
* The performance gradient falls below min_grad.
* Validation performance has increased more than max_fail times since the last time it decreased (when using validation).

The main aim of this study is to investigate the effect of Al_2O_3/ SiO_2, Na_2O/Al_2O_3, Na_2O/H_2O, and Na/[Na+K] on compressive strength of geopolymers. For this purpose and in this work, Traingda method was used as training algorithms to predict the compressive strength of geopolymers and early stopping was used to avoid the over fitting.

NETWORK ARCHITECTURE

After gathering more than fifty data it was preprocessed to increase the efficiency of the ANN training (Subaer, 2007 and Duxson, 2007). The preprocessing involved converting all input data into values between zero and one. A three-layer feed forward network is designed with chemical compositions of alumina silicate and alkali activators as inputs and compressive strength as output. Figure 1 shows the number of neurons in hidden layer and output layer are 5 and 1, respectively. Tan-sigmoid (tansig) function is selected as the hidden layer transfer function and the linear function is selected for output layer transfer function due to their ability to learn complex nonlinear relation between input patterns and output data.

The reduction of mean squared error (MSE) along the training interval shows that MSE converge to 0.9×10^{-1} and at this point the ANN was stopped to inhibit the over fitting problem. The calculated R values by comparing data with Y=X line are presented in Figure 2. With respect to the obtained results, it can be concluded that the predicted values of ANN for compressive strength shows good correlation with the real experimental values for both training and test data.

Table1. Training Data and predicted compressive strength (PCS) of geopolymer samples

Sample No.	SiO_2/Al_2O_3	Na_2O/Al_2O_3	Na/[Na+K]	H_2O/Na_2O	CS	PCS
10	4	0.8	1	10	2.3	37.20
15	4	1	1	10	2.74	38.27
2	2.5	0.6	1	10	6.6	9.17
11	2	1	1	10	8.23	8.24
15	2.3	1	0	11	8.94	11.30
6	2	0.8	1	10	12.09	14.02
30	2.3	1	0.75	11	12.62	14.09
25	2.3	1	0.5	11	13.81	12.24
35	2.3	1	1	11	15.79	16.04
54	3.8	1.14	1	17.5	25.03	29.60
43	4.4	1.2	1	11	26.62	23.39
53	3.55	1.04	1	20	27	25.19
40	4	1	1	15	30.02	41.69
7	2.5	0.8	1	10	30.56	24.98
45	3.9	0.95	1	12	32.57	41.47
44	3.05	0.7	1	11.42	33.43	36.30
52	4	1	1	11	33.86	39.07
12	2.5	1	1	10	34.19	31.63
41	4.2	1.1	1	11	36.57	32.69
46	3.5	0.75	1	14	37.93	40.82
50	3.5	1	1	11	38.44	50.02
36	2.8	1	1	11	38.93	47.31
48	3.63	1.04	1	12	39.05	42.63
42	3.5	1	1	9.3	40.55	51.52
16	2.8	1	0	11	46.07	45.98
21	2.8	1	0.25	11	47.16	46.68
31	2.8	1	0.75	11	48.71	51.15
26	2.8	1	0.5	11	49.71	48.17
8	3	0.81	1	10	52.36	53.54
37	3.3	1	1	11	57.91	55.20
5	4	0.6	1	10	59.11	45.28
14	3.5	0.98	1	10	60.22	52.36
29	4.3	1	0.5	11	60.73	74.86
17	3.3	1	0	11	65.9	72.01
39	4.3	1	1	11	66.83	36.15
34	4.3	1	0.75	11	71.02	69.17
9	3.5	0.805	1	10	74.09	54.49
22	3.3	1	0.25	11	74.41	72.47
24	4.3	1	0.25	11	75.66	72.45
32	3.3	1	0.75	11	77.68	75.76
23	3.8	1	0.25	11	78.78	75.72
38	3.8	1	1	11	81.6	42.45

Table1 (continue). Training Data and predicted compressive strength (PCS) of geopolymer samples

Sample No.	SiO_2/Al_2O_3	Na_2O/Al_2O_3	Na/[Na+K]	H_2O/Na_2O	CS	PCS
1	2	0.6	1	10	4.3	10.76
20	2.3	1	0.25	11	9.11	11.54
49	4.5	1.57	1	10.3	24.95	16.53
47	4.01	1.16	1	13.1	31.98	27.23
51	3.275	0.85	1	10.58	38.83	58.39
3	3	0.6	1	10	46.28	33.53
4	3.5	0.595	1	10	57.26	55.59
19	4.3	1	0	11	65.31	73.48
27	3.3	1	0.5	11	74.33	73.85
18	3.8	1	0	11	83.22	75.81

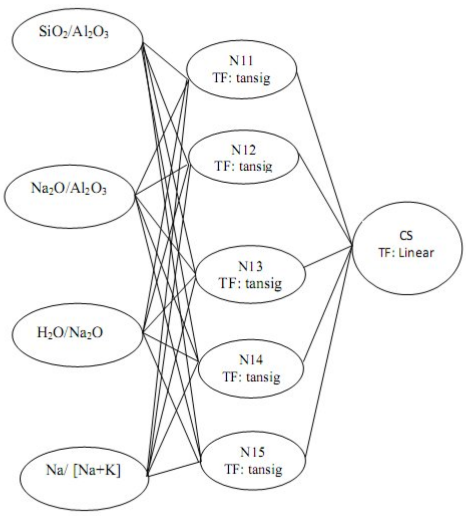

Figure1. Neural Network Arcitecture

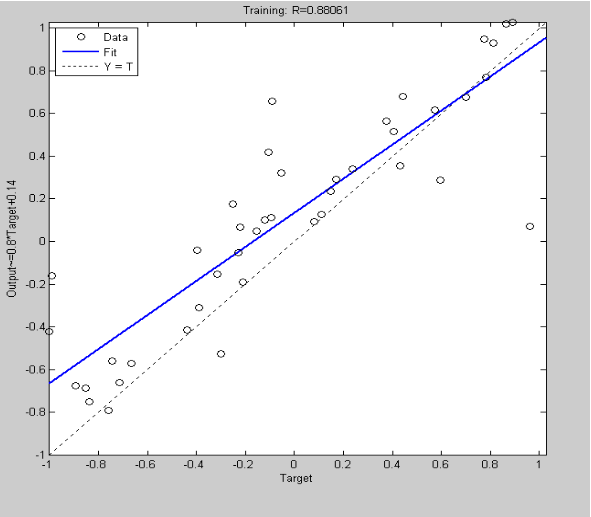

Figure2. Train and test data regression by comparing data with Y=X

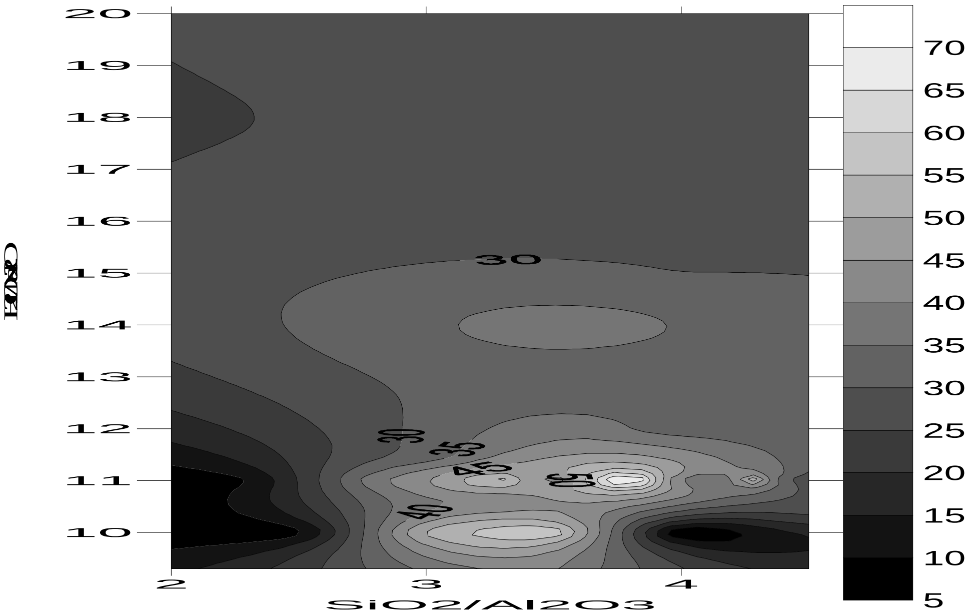

Figure 3(a). Contours plot of compressive strength that shows the effect of SiO_2/Al_2O_3 and H_2O/Na_2O on compressive strength (MPa)

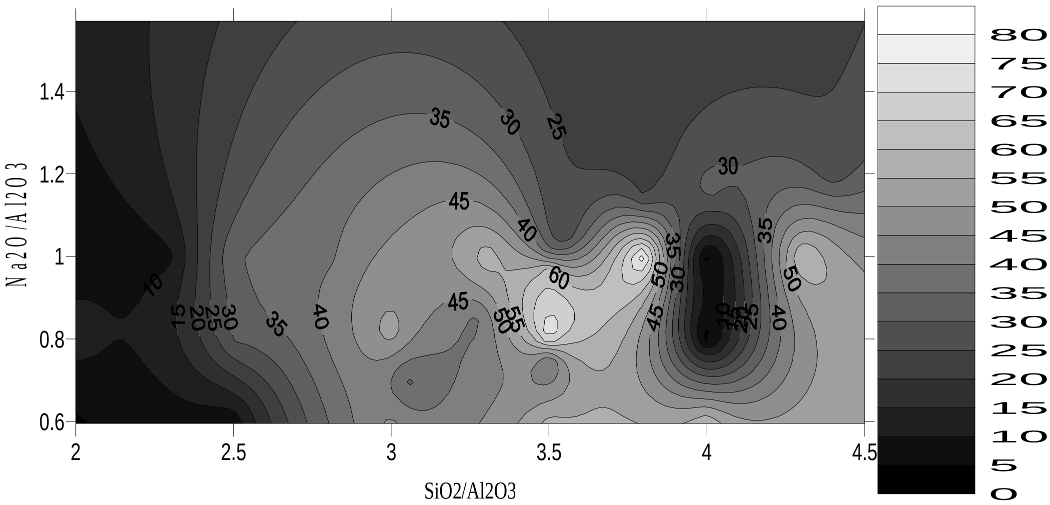

Figure 3(b). Contours plot of compressive strength that shows the effect of SiO_2/Al_2O_3 and Na_2O/Al_2O_3 on compressive strength (MPa)

DISCUSSION AND RESULTS

In this paper optimum chemical composition rages for producing geo-polymer cement and concrete with compressive strength of approximately 40 MPa was found.

Effect of SiO_2/Al_2O_3 on compressive strength:

Figures 3a and 3b show the effects of SiO_2/Al_2O_3 and H_2O/Na_2O on compressive strength of samples, respectively. Considering optimum ratios of other parameters, it can be seen that optimum value of SiO_2/Al_2O_3 is about 3.1 to 3.7. This follows the pattern reported in literature. Most researchers believe that with increasing SiO_2/Al_2O_3 ratio, polysialatesiloxo and polysialatedisiloxo structures become dominant which have more strength and stiffness in compare with polysialate structures. Thus the compressive strength is higher with increasing SiO_2/Al_2O_3 ratio. On the other hand solubility and gel formation decreases with increasing SiO_2/Al_2O_3 ratio, therefore the compressive strength of geopolymers tends to decrease in high SiO_2/Al_2O_3 ratios. In low SiO_2/Al_2O_3 ratios (<3.1), existence of coarse voids, in compare with finely distributed voids in high SiO_2/Al_2O_3 ratios (>3.7), is another reason for low compressive strength of the samples with that ratios. Superposition of these parameters affects the compressive strength of geopolymers and results an optimum range for SiO_2/Al_2O_3 ratios.

Effect of Na_2O/Al_2O_3 on compressive strength:

Figures 3b and 3a, considering optimum ratios of other parameters, show the effects of Na_2O/Al_2O_3 and SiO_2/Al_2O_3 on compressive strength of samples, respectively. It can be seen that the optimum values of Na_2O/Al_2O_3 ratio are 0.8 to 1.0. This follows theoretical principles of geopolymer formation mechanisms. Positive ions such as Na^+ must be present in the framework cavities to balance the negative charge of Al_3^+ in IV-fold coordination. Due to the fact that positive ions such as Na^+ partially are consumed to form Na_2CO_3, in low Na_2O/Al_2O_3 ratios, the amount of positive ions is not sufficient to balance the negative charges in low Na_2O/Al_2O_3 ratios. Therefore the geopolymer structure becomes distorted and without stability in low Na_2O/Al_2O_3 ratios and the optimum value of Na_2O/Al_2O_3 ratio is 0.8 to 1.0.

Effect of H_2O/Na_2O on compressive strength:

Figures 3d and 3b show the effects of H_2O/Na_2O and Na_2O/Al_2O_3 molar ratios on compressive strength of samples, respectively. From these figures it can observed that the optimum value of H_2O/Na_2O ratio is about 10 to 11 to achieve the structural compressive strength. In high ratios of H_2O/Na_2O the amount of OH^- is high which causes high amount of porosity and tends to decrease the compressive strength of geopolymer. On the other hand, water provides the suitable media for geopolymer reaction and in low ratios of H_2O/Na_2O the rate of geopolymer reaction is low. Therefore compressive strength of geopolymer decreases in low ratios of H_2O/Na_2O. Superposition of these mechanisms results the structural compressive strength in the optimum value of H_2O/Na_2O ratio which is equal to 10-11.

Effect of Na/[Na+K] on compressive strength:

Figures 3c and shows the effects of Na/[Na+K] and SiO_2/Al_2O_3 on compressive strength of geopolymer, respectively. It can be seen that in lower SiO_2/Al_2O_3 molar ratios, optimum value of Na/[Na+K] ratio is about 1, whereas in higher molar ratios of SiO_2/Al_2O_3, the optimum value decreases up to 0.6. The result follows the results achieved by Duxson et al. (Duxon, 2005, and 2007). They believed that K^+ ions are more active than Na^+ ions and potassium is preferentially incorporated in to the formation of geopolymeric gels. Thus in lower amount of SiO_2/Al_2O_3 molar ratios, samples containing potassium has lower level of SiO_2/Al_2O_3 and less compressive strength. This phenomenon was called Mixed Alkali Effect in the formation of geopolymer by Duxson (Duxon, 2005, and 2007).

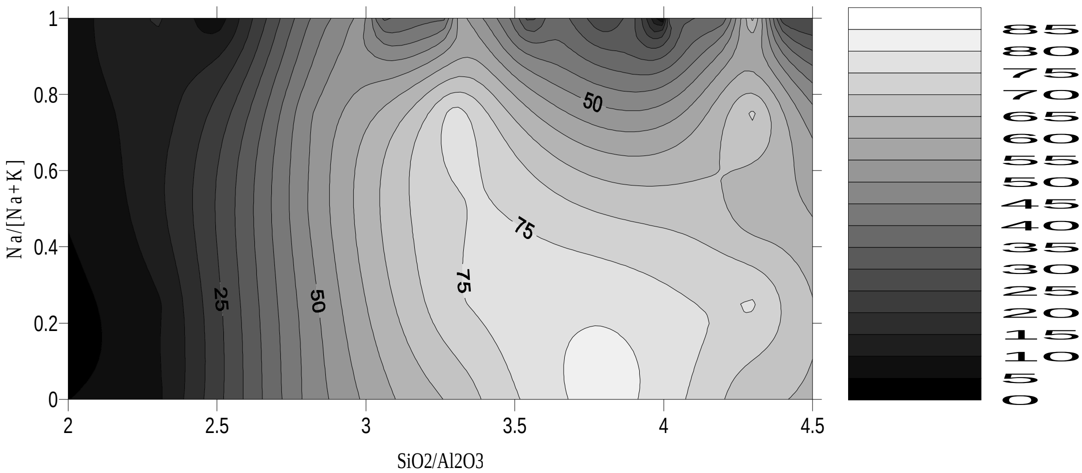

Figure 3(c). Contours plot of compressive strength that shows the effect of SiO_2/Al_2O_3 and Na/[Na+K] on compressive strength (MPa)

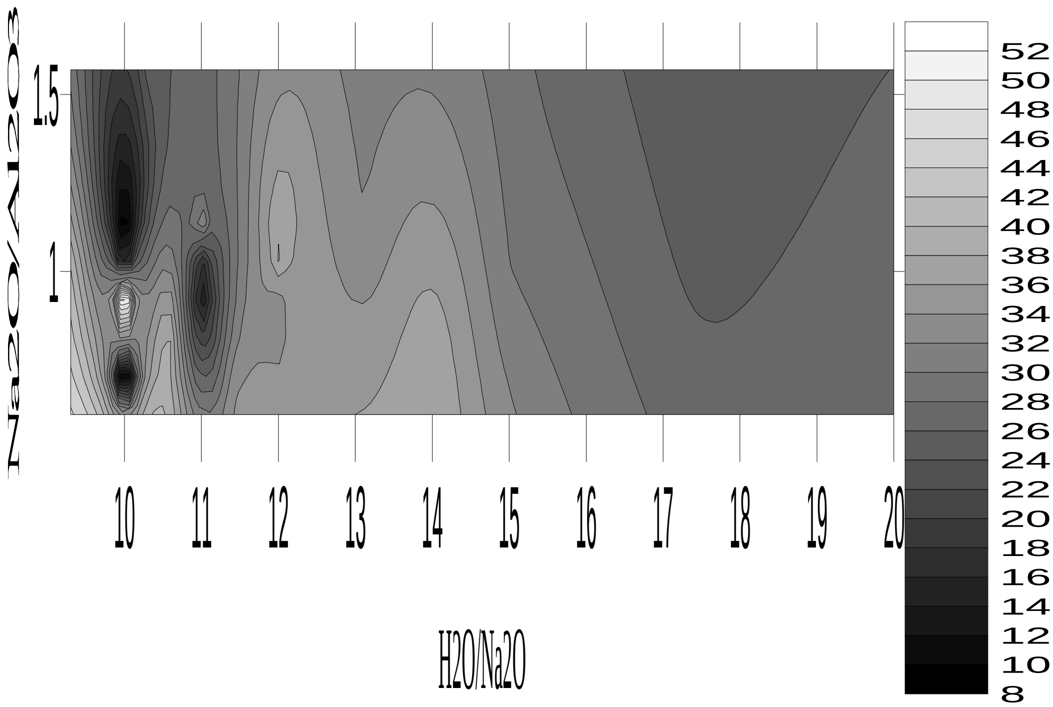

Figure 3(d). Contours plot of compressive strength that shows the effect of H_2O/Na_2O and Na_2O/Al_2O_3 on compressive strength (MPa)

CONCLUSION:

1. Neural network method can be useful to predict compressive strength of geopolymer concrete.

2. A three-layer feed forward network with tan-sigmoid function as the hidden layer transfer function and the linear function as output layer transfer function can be an optimum network architecture to predict compressive strength of geopolymer concrete.
3. The results showed the optimized ranges of ratios SiO_2/Al_2O_3, Na_2O/Al_2O_3, H_2O/Na_2O and Na/[Na+K] to achieve more than target compressive strength which is 40Mpa at 28 days, should be 3.1-3.7, 0.8-1.0, 10.0-11.0, and 0.6-1.0, respectively.

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