Using Artificial Neural Networks for the Prediction of the Compressive Strength of Geopolymer Fly Ash

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Abstract-Geopolymers are promising cement replacement materials as their use results in a considerable reduction of CO2 emissions. Geopolymer Fly ash (GF) is a widely used geopolymer due to its low cost and waste management achievement. The compressive strength of GF depends on variables such as curing time, curing temperature, NaOH molarity, the ratio of sodium silicate to sodium hydroxide, the ratio of fly ash to alkaline solution, etc. Artificial Neural Networks are employed to predict the strength of GF due to their accurate prediction capability as well as saving time and cost of experimental work. The obtained Root Mean Square Error (RMSE) and correction coefficient (R2) values were 4.47 and 0.972 respectively. The results illustrate the ability of the ANN model to be used as an efficient tool in predicting the compressive strength and determining the optimal values of GF parameters. The maximum strength of GF was observed for 2 hours curing time at 100°C, molarity of 10, fly ash to alkaline solution ratio of 3, and sodium silicate to sodium hydroxide ratio of 1.

Keywords-fly ash; alkaline solution; geopolymer fly ash; Artificial Neural Networks (ANNs); compressive strength

I. INTRODUCTION

Climate warming is a serious global issue. The main reasons for climate warming are human activities that result in changes in the concentration of greenhouse gases such as CO_2 in the atmosphere [1]. One of the main sources of greenhouse gas emissions is the construction industry. The cement used in the construction sector produces significant amounts of CO_2 [2]. Therefore, the replacement of cement with eco-friendly alternatives such as fly ash, rice husk ash, and GGBS can significantly reduce the amount of CO_2 emissions [3-7].

Geoplymers are a new cement replacement material with promising performance for cement with less greenhouse gas emissions [8]. Geopolymer binders are produced through the reaction of aluminosilicate materials with alkaline solution. Fly ash, metakaoline, and ground granulated blast furnace slag are the most commonly used aluminosilicate materials. High strength is obtained with fly ash-based geopolymers [9]. Sodium hydroxide and sodium silicate or potassium hydroxide and potassium silicate mixtures are the most commonly used alkaline solutions [7]. Equations (1) and (2) explain the geopolymer material forming mechanism [10, 11]. The water expelled during the chemical reaction leaves as nano-pores in the mix during curing time and imparts workability to the geopolymer mix during handling [12].



Investigating the mechanical properties of geopolymer materials by conducting experiments is time consuming and costly. There are many factors affecting the strength properties of geopolymers which make difficult their accurate estimation [13]. Mechanical modeling, analytical modeling, statistical methods, and artificial intelligence are the various methods used for the prediction of the strength properties of concrete [14]. Artificial intelligence is the most extensively used method for the prediction of the compressive strength of concrete. The use of ANNs is the most popular and widely used method in the area of artificial intelligence due to its easiness and prediction accuracy [15]. ANN modeling is a powerful machine learning technique that can solve various scientific problems [16]. In civil engineering, ANNs are widely used to predict the mechanical properties of concrete.

The compressive strength of concrete incorporated with fly ash admixture was predicted with Gene Expression Programming (GEP), ANNs, and Decision Tree (DT) algorithm in [17]. Softcomputing tools such as ANNs, Response Surface Methodology (RSM), and GEP have been applied to predict and analyze the compressive strength of alkali-activated strain-hardening geopolymer composites in [18]. The effect of parameters such as curing time, Ca(OH)₂ content, amount of superplasticizer, NaOH concentration, mould type, geopolymer type, H₂O/Na₂O molar ratio, etc. on the compressive strength of different types of geopolymers were analyzed with ANNs in [9]. The influence of

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sodium silicate to sodium hydroxide ratio and fly ash to alkaline solution ratio on the compressive strength of fly ash-based geopolymers was assessed using ANNs in [19]. Studies including the prediction of compressive strength of cement-based materials and geopolymer composites using ANNs are [20, 21].

In this study, ANNs are used to determine the compressive strength of geopolymer fly ash. Parameters such as NaOH molarity, Na₂SiO₃/NaOH ratio, fly ash/alkaline solution ratio, curing temperature, and curing time influence the compressive strength of geopolymer fly ash. Parameter optimization is conducted using ANNs.

II. EXPERIMENTAL PHASE

A. Materials

Fly ash, sodium hydroxide (NaOH), and sodium silicate (Na₂SiO₃) solutions were used. The fly ash was collected from Mettur Thermal power plant, Tamilnadu, India and industrial grade chemicals Na₂SiO₃ and NaOH pellets were collected from coimbatore, Tamilnadu. The fly ash was class-F based on its chemical composition [22]. The specific gravity of fly ash was determined in accordance with IS1727 [23] and the value 2.12 was obtained. The chemical composition of Na₂SiO₃ solution used is SiO₂=32.2%, Na₂O=14.01% and H₂O =53.79% by mass.



Fig. 1. Geopolymer fly ash cubes.

B. Sample Preparation and Testing

Sodium hydroxide solution and sodium silicate solution were mixed to prepare the alkaline solution. The alkaline solution was prepared one day before it was mixed with fly ash. Fly ash and alkaline solution were mixed and Geopolymer Fly ash (GF) cubes of 70.6mm×70.6mm×70.6mm were cast. The GF cubes were subjected to oven curing and were demolded. The compressive strength was tested after one day by keeping the cube specimens at room temperature. Figure 1 shows the Geopolymer Fly ash cubes ready for testing. The five considered parameters and their values are:

- Curing temperature: 50°C, 75°C, 100°C, 125°C, 150°C
- Curing time: 1hr, 2hr, 3hr
- Fly Ash/Alkaline Solution ratio (FA/AS): 2.5, 3, 3.5, 4
- Na₂SiO₃/NaOH ratio: 1, 1.5, 2, 2.5
- Molarity of NaOH: 6M, 8M, 10M, 12M

III. MODELING PHASE

ANNs are used in this study to predict the compressive strength of GF.

A. Artificial Neural Networks

ANNs are a widely employed method in different fields of artificial intelligence [24]. ANNs are powerful machine learning methods for predicting and solving different scientific computations [16]. ANNs are widely used in the area of civil engineering for predicting concrete's mechanical properties. ANN modeling consists of two steps: 1) Network training with the available training data set and 2) the trained network is tested to compute the prediction accuracy.

B. Neural Network Model

A Back Propagation Network (BPN) was used in this study to train the ANN model. The BPN training set consists of two stages, the feed forward stage and the back propagation stage. In the feed forward stage, the input node is transferred by the input layer neurons to hidden layer neurons. Each hidden layer neuron calculates the weighted sum of its input, and the sum is transferred through its activation function and the activation value is given to the output layer. The output layer neurons compute the weighted sum of each neuron and the sum is transferred through its activation function, forming the network output value. The sigmoidal function is generally used as activation function. The output is given by:

$$f_{j} = \frac{1}{1 + \exp\left(-\sum w_{ji}o_{i} + b\right)}$$
(3)

where: w_{ji} is the connection weight from the lower layer neuron *i* to the upper layer neuron *j*, o_i is the output of the neuron *i*, and *b* is the bias value. In the second stage, the output layer transfers the network error to the input layer, and the network error is minimized to an acceptable level by adjusting the weights.

The utilized network consists of 5 neurons in the input layer, 5 neurons in the hidden layer, and 1 neuron in the output layer. The hidden neurons are arranged in 2 hidden layers to reduce the error percentage. Table I lists the ANN model parameters. The input layer consists of curing temperature, curing time, fly ash to alkaline solution ratio, sodium silicate to sodium hydroxide ratio, and NaOH molarity and the output layer represents the Compressive Strength (CS) of GF. The data set for preparing ANN model includes 63 experimental results provided in Table II. The ANN prediction accuracy is validated using 66% of the data for training and the remaining data for testing.

TABLE I. ANN MODEL PARAMETERS

Parameter	Value
Number of inputs	5
Number of hidden layers	3
Number of hidden layer units	8
Number of outputs	1
Network architecture	BPN
Training function	Sigmoidal function
Number of training	62
Number of testing	21

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Sample No	Curing temperature (°C)	Curing time (hr)	FA/AS	Na ₂ SiO ₃ /NaOH	NaOH molarity	CS (N/mm ²)
1	50	1	3	2	10	0
2	50	2	3	2	10	0
3	50	3	3	2	10	0.71
4	100	1	3	2	10	4.50
5	100	2	3	2	10	25.08
6	100	3	3	2	10	24.28
7	150	1	3	2	10	7.50
8	150	2	3	2	10	21.16
9	150	3	3	2	10	0
10	100	2	2.5	2	10	6.76
11	100	2	3	2	10	25.08
12	100	2	3.5	2	10	22.28
13	100	2	4	2	10	11.33
14	100	2	3	1	10	28.25
15	100	2	3	1.5	10	31.47
16	100	2	3	2	10	25.08
17	100	2	3	2.5	10	17.48
18	100	2	3	1	8	14.64
19	100	2	3	1.5	8	23.43
20	100	2	3	2	8	17.19
21	100	2	3	2.5	8	14.10
22	100	2	3	1	12	22.07
23	100	2	3	1.5	12	28.44
24	100	2	3	2	12	25.46
25	100	2	3	2.5	12	22.21
26	50	1	3	1.5	10	0
27	50	2	3	1.5	10	0
28	50	3	3	1.5	10	2.95
29	100	1	3	1.5	10	2.90
30	100	2	3	1.5	10	31.47
31	100	3	3	1.5	10	30.27
32	150	1	3	1.5	10	9.71
33	150	2	3	1.5	10	26.22
34	150	3	3	1.5	10	0
35	100	2	2.5	1.5	10	13.09
36	100	2	3	1.5	10	31.47
37	100	2	3.5	1.5	10	30.29
38	100	2	4	1.5	10	20.02
39	75	2	3.5	1.5	12	5
40	100	2	3.5	1.5	12	26.4
41	125	2	3.5	1.5	12	32
42	150	2	3.5	1.5	12	30.5
43	125	1	3.5	1.5	12	16.7
44	125	2	3.5	1.5	12	27.1
45	125	3	3.5	1.5	12	26.2
46	125	2	3.5	1	12	17.5
47	125	2	3.5	1.5	12	21.5
48	125	2	3.5	2	12	20.2
49	125	2	3.5	2.5	12	16.8
50	100	2	1	3	6	25.9
51	100	2	1.5	3	6	23
52	100	2	2	3	6	18.33
53	100	2	2.5	3	6	11.59
54	100	1	1	3	8	2.2
55	100	1	1.5	3	8	9.1
56	100	1	2	3	8	4.2
57	100	1	2.5	3	8	3.8
58	100	1	1	3	10	11.5
59	100	1	2.5	3	10	4
60	100	1	1	3	12	11.8
61	100	1	1.5	3	12	9.5
62	100	1	2	3	12	3.8
63	100	1	2.5	3	12	3
55	100	1	2.5	5	1 12	5

TABLE II.ONE DAY CS TEST RESULTS FOR GF CUBES

IV. RESULTS AND DISCUSSION

A. Test Results

1) One Day Compressive Strength

The CS of the GF cubes was determined by following the ASTMC109 [25]. The one day compressive strength of 10M GF with different curing temperatures and curing times was obtained as shown in Figure 2. The GF cubes after 1 and 2hr of curing time at 50°C curing temperature were observed in wet condition and no strength was obtained. The strength was increased with rise in temperature and the maximum compressive strength of GF was observed for 100°C curing temperature. Similar results were reported in [26-28]. When the curing temperature became more than 100°C, a gradual decrease in strength was noticed. The curing time also showed influence on compressive strength and the maximum strength was observed for 2hrs curing time. Hence, the maximum value of 31.47N/mm² of strength was obtained for 100°C and 2hr curing time.



Fig. 2. One day compressive strength of GF with curing temperature and curing time.



Fig. 3. One day compressive strength of GF with FA/SA ratio.

The one day compressive strength of 10M GF with different FA/AS ratios is shown in Figure 3. The FA/AS ratio was increased by 0.5 at 100°C curing temperature and 2hrs curing time. The maximum strength of GF was observed at the ratio of 3 as 31.47N/mm². The strength decreases beyond FA/AS ratio of 3. The one day CS of GF with different sodium silicate to sodium hydroxide ratios and NaOH molarities is shown in Figure 5. The maximum strength was observed for

Na₂SiO₃/NaOH ratio of 1 for every molarity. An increase in CS was observed with increase in molarity due to the increase of Na⁺ ions which enhance the geopolymer reaction [29, 31]. Maximum strength was observed in 10M GF cubes. Similar results were reported in [26-28]. When the molarity became more than 10M, a decrease in strength was observed due to the increase in the amount of OH⁻ ions which reduce the geopolymer reaction [26].



Fig. 4. The one day compressive strength of GF with curing temperature and curing time.



Fig. 5. Comparison between the ANN model predicted data and the experimental data.

B. Modeling Results

The most important step in ANN model development is the ANN architecture determination which suits the real problem. The ANN architecture L-5-4-3-1-1 was finalized after trial and error process. The performance of the ANN model was checked with the performance measures Root Mean Square Error (RMSE) and correction coefficient (\mathbb{R}^2) between the experimental results and the predicted results. They were computed by (4) and (5):

$$RMSE = \sqrt{\frac{\sum (x_i - y_i)^2}{n}}$$
(4)

where x_i is the target value, y_i is the predicted value, and n is the number of test data.

TABLE III. EXPERIMENTAL AND PREDICTED BALUES

Experimental CS (N/mm ²)	ANN CS (N/mm ²)
0.71	1.14
7.5	18.7
23.43	18.54
28.25	25.17
17.48	24.15
22.07	26.014
22.21	25.98
2.9	5.06
25.66	26.08
22.32	25.03
26.4	26.08
16.7	24.01
16.8	24.01
3	3.98
1.9	0.234
4.1	4.06
5.9	7.74
13.8	5.3
11.5	6.82
5.2	9.87
1	0
14.1	14.5

Figure 5 represents the ANN model predicted data and the experimental data for the one day compressive strength test. The experimental compressive strength values and the corresponding ANN model predicted compressive strength values are given in Table III. The accuracy of the prediction is indicated by RMSE and R^2 . The RMSE and R^2 obtained values were 4.47 and 0.972 respectively, which show that the ANN is effective in the prediction of the CS of GF.

V. CONCLUSIONS

This study studies various factors affecting the compressive strength of geopolymer fly ash. The geopolymer fly ash was produced by mixing alkaline solution and fly ash. The factors considered in this study were curing temperature, curing time, fly ash to alkaline solution ratio, sodium silicate to sodium hydroxide ratio, and the molarity of sodium hydroxide. ANNs were employed in this study to predict the compressive strength of GF and the prediction accuracy was validated.

- The selected values of curing temperature were: 50, 75, 100, 125, and 150°C. The maximum compressive strength was observed at 100°C curing temperature.
- The values of curing time were as 1, 2, and 3hr. The maximum compressive strength was observed for 2hr curing time.
- The fly ash to alkaline solution ratio was 2.5, 3, 3.5, and 4. The maximum compressive strength was obtained for ratio equal to 3.

• The Na₂SiO₃/NaOH ratio was selected as 1, 1.5, 2, and 2.5. The maximum compressive strength was obtained for the ratio of 1.

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- The molarity of NaOH varied as 6, 8, 10, and 12. The maximum compressive strength was obtained for 10M geopolymer fly ash.
- An ANN was developed to predict the compressive strength of GF. The accuracy of the model was evaluated with RMSE and R². The obtained values were 4.47 and 0.972 respectively. These values of RMSE and R² confirm that the utilization of ANN for the prediction of the compressive strength of GF is a good choice due to its excellent correlation with the experimental results. This study suggests that ANNs are an effective tool in strength prediction of GF, reducing further the experimental cost and time.
- The geopolymer fly ash with its optimized parameters provides sufficient strength. Hence, it is applicable as a cement replacing material in concrete.

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