A Computational Approach to Investigate the Properties of Geopolymer Concrete

B. Ramya Madhuri and K. Srinivasa Rao

1 Introduction

In this concrete era, research has been carried out to find out alternatives to conventional concrete. In this hunt for new materials, geopolymer concrete has emerged as one of the best alternatives for conventional concrete. Geopolymer concrete is a sustainable material as its production is pollution-free, unlike conventional concrete. This can be developed using precursor materials such as fly ash, Ground Granulated Blast Furnace Slag (GGBS), red mud, rice-husk ash, etc., which are silica-rich materials and industrial by-products. Moreover, it prevents the depletion of limestone as well as the emission of carbon dioxide.

Geopolymer concrete can be developed by combining the precursors and the hardeners. The hardeners such as sodium or potassium hydroxide in combination with sodium or potassium silicate can be used. The chemistry involved in the production of geopolymer concrete is quite different from that of conventional concrete. The synthesis of geopolymer involves the dissolution of alumina and silica oxides from the precursor materials under highly alkaline environment, transportation of the dissolved oxide minerals followed by coagulation and then finally polycondensation to form 3-D network of silico-aluminate structures [1]. This process involves the expulsion of water quite contrary to the hydration of cement in conventional concrete. The water present in the chemicals and the water which is expelled out is merely used to provide workability for the mix [2].

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Table 1 Properties of Alccofine 1203 (data as furnished by the manufacturer)

Property	Unit	Value
Average particle size	Microns	4–6
Fineness as specific surface	cm^2/gm	12,000
Specific gravity	–	2.86 ± 0.02
Bulk density	kg/m^3	600 to 700

Table 2 Chemical composition of Alccofine 1203 [3]

Constituents	Composition (%)
SiO_2	35.30
MgO	6.20
Al_2O_3	21.40
Fe_2O_3	1.20
SO_3	0.13
CaO	32.30

2 Experimental Programme

2.1 Materials

In this study, geopolymer concrete is prepared by using class F fly ash and Alccofine 1203 as the precursors. Class F fly ash is collected from NTPC Simhadri. Alccofine 1203 is a low-calcium silicate-based micro-fine mineral additive. The physical properties and chemical composition of Alccofine 1203 are listed in Tables 1 and 2, respectively. The hardeners used are sodium hydroxide and sodium silicate. Sodium hydroxide is available as solid flakes and sodium silicate is available in solution form. The modulus of sodium silicate (Na_2O—15%, SiO_2—34.5%) is approximately 2.3. It is the ratio of percentage composition of SiO_2 to Na_2O by weight.

2.2 Mix Design

The mix design is done as per IS 10262:2019, but in case of geopolymer concrete, the alkaline liquid–binder ratio is considered instead of the water–cement ratio [4]. Alkaline liquid or hardener refers to the mixture of sodium hydroxide and sodium silicate solutions. In addition to the alkaline liquid, extra water is also added to the geopolymer concrete mix to increase the workability of the mixture. Extra water is added based on water to geopolymer solid ratio, such that the total mass of water present in the mix is equal to the water contained in the sodium hydroxide and sodium silicate solutions and the extra water. Geopolymer solids refer to the binder (fly ash

Table 3 Geopolymer concrete mixture proportions

Materials	Mass (kg/m^3)
Fly ash (ASTM class F)	361
Alccofine 1203	19
Fine aggregate	726
Coarse aggregate	1224
Sodium silicate solution ($SiO_2/Na_2O = 2.3$)	91.2
Sodium hydroxide solution	60.8
Extra water	38.11

and Alccofine) as well as the solids present in sodium hydroxide and sodium silicate solutions [5].

The binder content of 380 kg is taken to develop an M30-grade geopolymer concrete. The alkaline liquid to binder ratio is 0.4 and water to geopolymer solid ratio of 0.3 is adopted after conducting several trials. The amount of total alkaline liquid required is computed and the quantities of NaOH and Na_2SiO_3 are determined based on their proportions. The mixture proportions for trial No. 4 are shown in Table 3.

2.3 Mixing, Casting and Curing

The sodium hydroxide solution with the required concentration should be prepared 24 h prior to the mixing so that the heat gets dissipated. And the sodium silicate solution is added to the sodium hydroxide solution 1 h before the mixing of concrete. This allows dissociation of silica in the solution which assists the process of geopolymerization. The geopolymer concrete is mixed using a pan mixer. Initially, the dry contents (binder and aggregates) are mixed well and then the hardener followed by the extra water is added gradually to the mix. The mixing time maintained is 6–8 min. The casting of specimens should be carried out within 2–3 min after mixing as the concrete mix gets stiffer with time and the workability decreases. The specimens are demoulded after 24 h and cured in ambient condition. Geopolymer concrete developed using only fly ash needs to be cured in an oven for 24 h maintaining the temperature at 60 °C, and this concrete exhibits low strength when cured in ambient condition. The addition of Alccofine accelerates the geopolymerization resulting in the development of strength even under ambient conditions. The trials were conducted by replacing fly ash with 30% Alccofine but it was found that the mix is too stiff to be handled and even its setting time is too low and cannot be mixed. It's getting hardened while mixing itself. This is due to the high percentage of Alccofine. Moreover, using higher percentages of Alccofine will result in increasing the cost of the concrete.

The compressive strength is determined by conducting the experiment on 150 × 150 × 150 mm cubes after 28 days of ambient curing as per IS 516–1959.

2.4 Taguchi Method of Optimization

Taguchi method of orthogonal arrays is an experimental methodology based on statistics, developed by Genichi Taguchi. Taguchi method is used to study the influence of various factors affecting the output of a process. In other words, it gives the mathematical relationship between input parameters and the response in any process. This method gives the S/N (signal/noise) ratio to evaluate the performance of the response. It is nothing but the ratio of the mean (signal) to the standard deviation (noise) [7]. The S/N ratio is also denoted by η. It is given by a loss function shown in Eq. (1):

$$\text{Larger the better S/N (dB)} = -10 \times \log_{10}\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{y_i^2}\right) \quad (1)$$

where $n =$ the number of times an experiment is performed and $y_i =$ the response or the output.

Taguchi method is used for its robustness. It is originated from fractional factorial method and in the more simplified form which can be easily applied to optimization problems. The number of experiments to be conducted is reduced considerably, when compared to methods such as full factorial method and response surface method. All the three variables can be varied at the same time unlike in one factor at a time method, reducing the number of experiments to almost one-third of the required. This saves time, resources, effort and money.

In this study, different mixes are prepared by varying the proportion of Alccofine in the binder, concentration of sodium hydroxide solution and the ratio of Na_2SiO_3 to NaOH. The percentage of Alccofine is varied from 0 to 25 with an increment of 5% in each trial. The concentration of NaOH taken is 8, 10 and 12 M. The ratio of Na_2SiO_3 to NaOH considered is 1.5, 2 and 2.5. By considering all these variations, the total number of experiments required to be conducted are 54 (6 × 3 × 3). The results of all the 54 trials can be predicted by conducting one-third (18) of the total number of experiments. Taguchi method of optimization is chosen to perform the parametric study on the geopolymer concrete. The different levels considered for the input parameters are shown in Table 4. The standard L18 orthogonal array design is developed in software 'Minitab 18' as shown in Table 5.

Table 4 Levels of the three factors

Factor	Symbol	Levels						Output parameters
		1	2	3	4	5	6	
Proportion of Alccofine	A	0	5	10	15	20	25	Compressive strength
Molarity of NaOH	M	8	10	12	–	–	–	
Ratio of Na_2SiO_3 to NaOH	R	1.5	2.0	2.5	–	–	–	

Table 5 Trials conducted as per Taguchi standard L18 array

Trial no	Alccofine proportion (%) (A)	Molarity of NaOH (M)	Ratio of Na_2SiO_3 to NaOH (R)	Compressive strength (Comp) (MPa)
1	0	8	1.5	8.74
2	0	10	2.0	12.22
3	0	12	2.5	10.67
4	5	8	1.5	28.00
5	5	10	2.0	19.34
6	5	12	2.5	24.74
7	10	8	2.0	31.23
8	10	10	2.5	32.67
9	10	12	1.5	42.96
10	15	8	2.5	37.04
11	15	10	1.5	40.89
12	15	12	2.0	50.67
13	20	8	2.0	58.00
14	20	10	2.5	46.07
15	20	12	1.5	60.00
16	25	8	2.5	65.33
17	25	10	1.5	75.56
18	25	12	2.0	58.67

3 Results and Discussions

The influence of all the three parameters, namely, proportion of Alccofine (A), molarity of NaOH (M) and the ratio of Na_2SiO_3 to NaOH (R) are graphically represented in Fig. 1. The three-dimensional surface plots are obtained as shown in Fig. 2.

From Figs. 1 and 2, it is clear that the compressive strength of the geopolymer concrete increases with an increase in the proportion of Alccofine in the binder. Alccofine is a micro-fine material so it helps in accelerating the rate of geopolymerization. Moreover, the addition of Alccofine to the binder allows the reaction to take place in ambient condition. It is clear that the proportion of Alccofine is the most influential factor among the three.

The average S/N values of all the factors at different levels are given in Table 6. The rank in the ninth column of Table 6 denotes the order of importance of the three factors. The factor with rank 1, i.e. the proportion of Alccofine is the most influential parameter among the three. And the ratio of Na_2SiO_3 to NaOH is the second most influential parameter among the three.

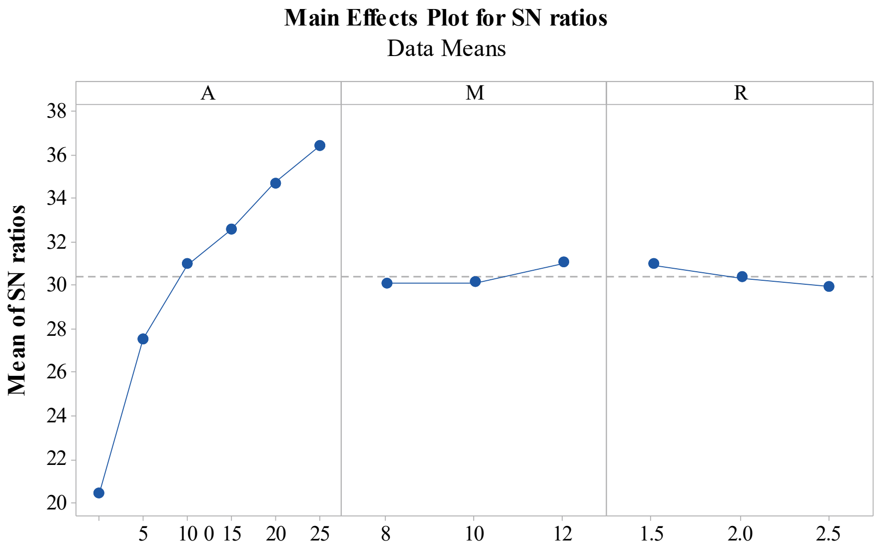

Fig. 1 Main effects plot for S/N ratios

The numerical value of the maximum point in each graph in Fig. 1 shows the optimum value or the best value of that particular parameter. The maximum S/N values are obtained at level 6 for 'A', at level 3 for 'M' at level 1 for 'R'. Therefore, the compressive strength of geopolymer concrete is maximum when the proportion of Alccofine is 25%, the concentration of NaOH is 12 M and the ratio of Na_2SiO_3 to NaOH is 1.5.

The objective of this study is to develop geopolymer concrete of M30 grade economically. The target strength of M30-grade concrete is 38.25, so the target strength is set at 38.25 MPa and the corresponding factors are determined. It is found that the target strength is achieved when the proportion of Alccofine is 12.5%, the concentration of NaOH is 9.02 M and the ratio of Na_2SiO_3 to NaOH is 2.0. The same is shown graphically in Fig. 3. The value of compressive strength can be obtained for all the values of factors within their constraints and for any specific value of compressive strength the values of three factors can be obtained. This is the advantage of optimization as this can be done without following the hectic experimental procedures. The required quantities are obtained by computation instead of experiments. The computation is performed by feeding the minimum required data to the program.

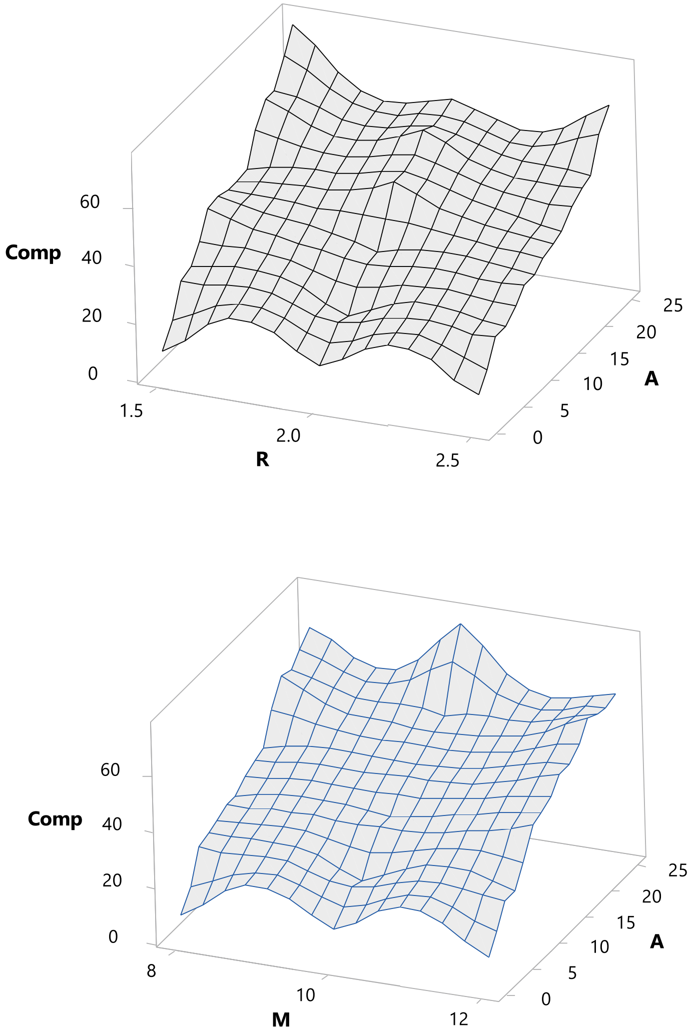

Fig. 2 3-D surface plots of compressive strength versus the input parameters

Table 6 Average S/N values of factors at different levels

	Average η (S/N) by factor level (dB)							
Parameter	1	2	3	4	5	6	Delta	Rank
Proportion of Alccofine	20.38	27.51	30.95	32.57	34.70	36.41	16.03	1
Molarity of NaOH	30.10	30.14	31.02				0.92	3
Ratio of Na_2SiO_3 to NaOH	30.97	30.35	29.94				1.02	2

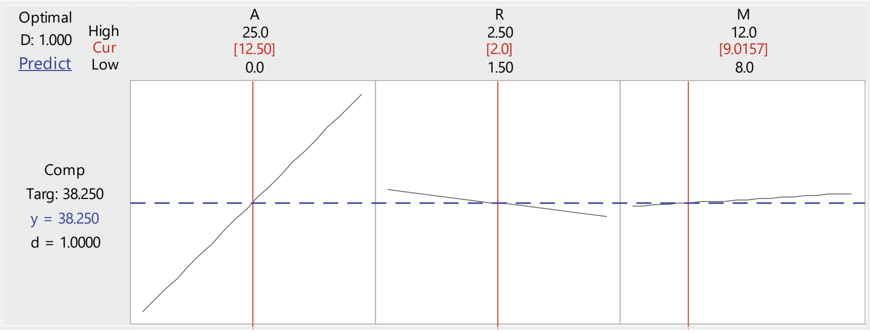

Fig. 3 Graph showing the factors at which target strength is obtained

3.1 Mathematical Modelling

The influence of all the input parameters on the response (compressive strength) can be predicted from Table 6 and also from the three-dimensional surface plots. However, a mathematical formulation of any phenomenon will serve better. The impact of the three input parameters on the response is mathematically formulated as shown in Eq. (2). The equation is developed by using regression analysis [8]. The linear regression curve is developed as it is the best fit for the available data.

$$\text{Comp} = 17.10 + 2.17\text{A} + 0.81\text{M} - 6.61\text{R} \tag{2}$$

The compressive strength can be computed for any values of A, M and R, within their constraints using Eq. (2).

4 Conclusion

The target strength for the M30-grade geopolymer concrete is obtained when the proportion of Alccofine is 12.5%, the concentration of NaOH is 9.02 M and the ratio of Na_2SiO_3 to NaOH is 2.0.

The results of present study are encouraging to achieve a sustainable concrete which can address the global issues such as disposal of huge quantities of fly ash and prevention of depletion of natural resources such as limestone. The usage of water can also be reduced as it is ambient cured.

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