Research Article

An Empirical Model for Geopolymer Reactions Involving Fly Ash and GGBS

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Numerous works are reported in literature regarding the enhancement of compressive strength of fly ash-GGBS geopolymer combinations with addition of alkali activators of varying concentrations. However, a limited study has been chronicled, revealing the specific role of alkali or alkaline earth contributed by the fly ash-GGBS combinations on the compressive strength development. It is well known that the strength of a geopolymer is dependent on gel formation from Al/Si ratio, Ca/Si ratio, and Ca/(Si + Al) ratio but their exact role when cured for various extended periods is unknown as yet. In the present study, alkali concentration in a fly ash-GGBS geopolymer combination was varied from 6 M to 12 M with increments of two mol in six different fly ash-GGBS combinations with a minimum of 20 percent and a maximum of 70 percent GGBS. The correlation coefficients between compressive strength and Al/Si, Ca/Si, and Ca/(Si + Al) ratios exhibited values higher than 0.95 taken individually. Multiple linear regression analysis with compressive strength (as dependent parameter) and individual values of Al/Si, Ca/Si, and Ca/(Si + Al) ratios (as independent parameters) was effectuated. It was observed that, depending on the composition, the compressive strength circumstantiated a changeover from Ca/Si to Ca/(Si + Al) ratio in the intermediate composition range. Such a detailed analysis is considered supportive of developing a suitable composition which will provide the optimum compressive strength of the combination.

1. Introduction

In alkali-activated geopolymer systems with calcium-containing solid alumina silicate sources, such as ground granulated blast-furnace slag (GGBS) and calcium fly ash (FA), rapid formation of C-A-S-H gels [1–3] (along with calcium in class C FA) resulting in quick setting [4, 5] has been reported. The C-A-S-H gel showed similar features like C-S-H gel presented in conventional OPC (ordinary Portland cement) concrete. Addition of soluble silicates is generally done into the alkaline activating solution for obtaining a rapid sol/gel transition with improved properties. Calcium has been attributed to the early age setting, which increases with time [6–8]. In the Na₂O–CaO–SiO₂–Al₂O₃–H₂O system, the coprecipitation of geopolymer gel due

to Si–Al–H and C–A–S–H has been found to have an exchange reaction where Na is replaced by Ca [9–11].

Regarding the role of Ca on the metakaolin based geopolymers, Chen et al. [10] suggested that the addition of Ca in metakaolin resulted in faster geopolymer gel formation leading to faster setting time and that there is evidence of C–A–S–H formation. These conclusions were supported by NMR (nuclear magnetic resonance) studies. Pulgalia and Mondal [11] indicated that in calcia-based systems, the phase characterization becomes difficult because of the coexistence of C–A–S–H, (C(N, K)–A–S–H), and (N, K)–A–S–H in the reaction products of fly ash-metakaolin geopolymers containing soluble form of calcium. They further suggested that conventional FTR analysis provided vibrations from initial

unreacted slag and calcium silicate hydrate and an overlapping pattern which is similar to OPC sample patterns. They resorted to conventional selective acid dissolution technique but also suggested that they could not differentiate between N-A-S-H and C-S-H gels.

1.1. Geopolymer Paste Modelling in Literature. Previous attempts using numerical modelling to investigate the geochemical reactions in the polymerization of fly ash-GBS geopolymer combinations included that by Dao et al. (2019) [12], which estimated the compressive strength of geopolymers using numerical methods (neural networks and genetic algorithms) to find an optimum mix design. Dao et al. (2019) [12] also showed that their models have strong potential for predicting the 28-day compressive strength and suggested that the modelling would help in reducing the time and cost of laboratory tests in the optimal design of geopolymer. Yadollahi et al. (2015) [13] estimated the compressive strength of geopolymer concrete using artificial neural networks (ANN) method and found that parameters including silica modulus, Na₂O content, water/solid ratios, and curing time can affect the compressive and tensile strengths of geopolymer concrete. Naseri et al. (2017) [14] estimated the results of compressive strength of concrete using SVM (Support Vector Machine). Nano-CuO was added at different content levels in self-compacting concrete and CuO effects were determined. Khotbehsara et al. (2018) [15] estimated the compressive strength of concrete with SnO₂, ZrO₂, and CaCO₃ nanoparticles. Both SVM (Support Vector Machine) and ANFIS (adaptive neurofuzzy interface system) were used to analyze the results. Badarloo et al. (2018) [16] estimated the relationship between compressive and tensile strengths of concrete using MATLAB software and probabilistic methods, and the error estimated with the experimental data was found to be nil. Awoyera et al. (2020) [17] included mechanistic properties including slump flow and funnel flow in a machine learning model for self-compacting geopolymer concrete. However, the model had not been tested in full commercial production of geopolymer concrete.

For more mechanistic-based modelling, Zhang et al. (2018) [18] produced theoretical models of geopolymer gels and found them to be close to those produced experimentally using computer simulation through MD (Molecular Dynamics) models with Si/Al molar ratios of 2 and 3. The simulation was carried out at temperatures ranging from 650 to 1800 K and the effect of Si/Al ratio and temperature on the polymerization process and the properties of computationally synthesized geopolymer gels were investigated. Cui et al. (2020) [19] compared the flexural behaviors of OPC and geopolymer concretes using Abaqus modelling. Using data obtained from testing and the literature, empirical equations were derived to describe the nonlinear correlation between the compressive strength and elastic modulus of fly ash based geopolymer concrete (CFGPC). They observed that the suggested formula had a reasonably high R² value of 0.7663, and when the variations in density were added to the regression analysis, R²

increased to 0.8652. Ling (2019) [20] observed the role of SiO₂/Na₂O mole ratio in alkaline solution, alkaline solution concentration in mass percent, and liquid-to-fly ash mass ratio (L/F). Ling observed using artificial neural network (ANN) that the curing temperature and time had significant influences on the setting time, compressive strength, and heat of geopolymerization which are critical properties for a concrete binder. It was concluded that the optimum mix design parameters result in favourable fly ash geopolymer properties (i.e., compressive strength, setting time, and heat generation). By using both Levenberg-Marquardt and Bayesian regularization algorithms, Siva Krishna and Ranga Rao (2019) [21] were able to use ANN models to predict the mechanical properties such as compressive, split tensile, and flexural strength values of concrete and observed that the Levenberg-Marquardt algorithm gave more accurate results than the Bayesian model. Finally, Mehdizadeh et al. (2018) [22] used a statistical experimental design based on response surface methodology (RSM) on an alkali-activated phosphorus slag to predict and optimize the compressive strength of different ages (3, 7, and 28 days). In their study, the binder samples were prepared with different molar ratios of SiO₂/Na₂O (S/N), Na₂O/Al₂O₃ (Na/Al), and H₂O/Al₂O₃ (H/Al) as alkali activators and the results showed that S/N molar ratio had a significant effect on 7 and 28 days of compressive strength. On the other hand, H/Al molar ratio was found to have the most significant effect on compressive strength when compared to other parameters. They concluded that RSM models were statistically adequate and could be used to predict the compressive strength.

1.2. Significance of Research. As per literature, Al/Si ratio, Ca/Si ratio, and Ca/(Si + Al) ratio in combinations may have a critical role to play in the development of compressive strength of the geopolymer system containing calcium and alkaline activators that are responsible for initiating polymeric reactions. Depending on the CaO/SiO₂ ratio, Al₂O₃/SiO₂ ratio, and CaO/(Al₂O₃ + SiO₂) ratio, the composition and properties of the gel may change and may affect the overall compressive strength of the product. In this paper, an attempt of using an empirical approach to establish the correlations is reported.

In the current study, the focus is also on the material transition; geopolymers have displayed compressive strengths comparable to the compressive strengths of Portland cements and with additional benefits of high temperature resistance and stability under acid attack. The setting of geopolymers, however, is closely associated with the transition from fluid to solid which can be accelerated with the addition of calcium. Calcium was found to decrease the Al/Si ratio for geopolymer formation, in particular the Al-substituted calcium silicate hydrate (C-A-S-H) formation and also the calcium silicate hydrate (C-S-H) formation. When compared to noncalcium mixes which are controlled by Al/Si ratios in normal geopolymer gel, calcium mixes experienced faster dissolution with higher compressive strengths.

It has been suggested that, with calcium addition, the gel substantially accelerated the setting behavior and the formation of (C-S-H) and (C-A-S-H) gels has caused the enhanced dissolution of the source material precursors.

In the current study, NMR tests showed that comparable amount of geopolymer gel existed at setting for both calcium and noncalcium mixes, which suggested that the geopolymer gel was partially responsible for the setting process. Since faster geopolymer gel formation was caused by faster dissolution, which yielded more Al and lowered the Al/Si for geopolymer gel formation (as confirmed by quantitative analysis using both ^{29}Si and ^{27}Al NMR spectroscopy), the lower Al/Si ratio can be considered to be sufficient to cause the significantly different setting behaviors. Furthermore, calcium consumes Si in the solution, which has been proven from indirect experiment and simulation.

In synthetic (C-S-H), a low Ca/Si ratio leads to high dissolved silica concentrations and low calcium concentrations, while at high Ca/Si ratio and in presence of high pH of 12.5 high calcium and low silica are typically measured. In (C-S-H) with a $\text{Ca/Si} \geq 1$, the aluminum uptake in (C-S-H) depends on the total amount of aluminium present in the sample and a close relation between aqueous aluminium concentrations and the molar Al/Si ratio in C-A-S-H is observed up to an Al/Si of approximately 0.1 (10, 12).

It should be noted, however, that the experimental samples prepared are based on synthetic materials that are not as complicated as commercial samples and do not represent the actual conditions of commercial products, and therefore it is logical to conclude that the above-mentioned observations may occur concurrently as the reaction proceeds with prolonged curing period. Furthermore, any change in the strength of the samples is an indirect measurement of the different phase formations and is an approximate representation of the dynamic situation, controlled by Si-Al-Ca-Na complex association in different stages of reaction, in actual commercial productions. Thus, the dynamic situations prevailing in geopolymer reactions with time cannot be compared with reported static experimental conditions in actuality. However, application and help of both correlation coefficients and multiple linear regression analysis together are definite indicators of the validity of the assumptions and scientific observations made in real-life situations.

The scientific communities have relied on the help of statistical correlations between two observations to establish the direct proof of the dependence/independence of the

observations; and, in time-dependent events, multiple linear regression analyses have been the means to establish the correlation between different temporal events. For the current study, a similar approach is used.

1.3. Theory. If a number of samples (A to G, Table 1) are related to the dependent variable (Y) and independent variables A, B, and C (as shown in the table), then the relationship can be expressed as

$$Y = [K1 (A)^{N1}] \times [K2 (B)^{N2}] \times [K3 (C)^{N3}], \quad (1)$$

where Y1 to Y6 are dependent variables (for different sets of experimental data points) related to the independent experimental variable parameters A (A1 to A6), B (B1 to B6), and C (C1 to C6).

Here, K1, K2, and K3 are proportionality constants in the correlation relationship between different Y and X values:

$$Y \propto (A)^{N1} \text{ or } Y = K1 (A)^{N1}, \quad (2)$$

$$Y \propto (B)^{N2} \text{ or } Y = K2 (B)^{N2}, \quad (3)$$

$$Y \propto (C)^{N3} \text{ or } Y = K3 (C)^{N3}. \quad (4)$$

These may be generalized as

$$Y = [K1 (A)^{N1}] \times [K2 (B)^{N2}] \times [K3 (C)^{N3}]. \quad (5)$$

In equation (2), if $N1 = 1$, then the equation exhibits a perfect linear relationship. In actual experiments, it is conventional to plot $\ln(Y)$ versus $\ln(A)$ values and to observe if the data points follow a linear relationship indicating high correlation between the variables. Similar regression plots between $\ln(Y)$ (Y1 to Y6) and $\ln(B)$ (B1 to B6) and $\ln(C)$ (C1 to C6) can be made to examine the correlations. A very high correlation coefficient (nearly one) is indicative of an excellent relationship between the dependent and independent variables.

From equations (2)–(5), the following modified expressions can be determined:

$$\begin{aligned} \ln(Y) &= \ln(K1) + N1 \ln(A), \\ \ln(Y) &= \ln(K2) + N2 \ln(B), \\ \ln(Y) &= \ln(K3) + N3 \ln(C). \end{aligned} \quad (6)$$

And

$$\ln Y = \{\ln(K1) + N1 \ln(A)\} + \{\ln(K2) + N2 \ln(B)\} + \{\ln(K3) + N3 \ln(C)\}. \quad (7)$$

Or

$$\ln Y = [\ln(K1) + \ln(K2) + \ln(K3)] + N1 \ln(A) + N2 \ln(B) + N3 \ln(C). \quad (8)$$

Or

$$[\ln Y - [\ln(K1) + \ln(K2) + \ln(K3)]] = N1 \ln(A) + N2 \ln(B) + N3 \ln(C)]. \quad (9)$$

The values of $\ln(K1)$, $\ln(K2)$, and $\ln(K3)$ can be ascertained from the intercepts on the Y-axis from individual $\ln(Y)$ versus $\ln(A)$ values, $\ln(Y)$ versus $\ln(B)$ values, and $\ln(Y)$ versus $\ln(C)$ plots.

Equation (9) is modified into multiple linear regression analyses and consists of solving algebraic equations with three unknown parameters. Furthermore, the Y values are modified as $[\ln(Y) - [\ln(K1) + \ln(K2) + \ln(K3)]]$ values. The numerical values of different modified Ys ($Y1$, $Y2$, $Y3$, etc.) are equated to the different A, B, and C values in the multiple linear regression analysis.

If there are a number of experimental data points (A, B, C, D, E, F, and G), then the individual graphs can be made with $\ln(Y)$ ($Y = Y1, \dots, Y6$) versus $\ln(A)$ ($A = A1, \dots, A6$) to determine the correlation coefficient values between Y and A. Similar plots can also be made with $\ln(Y)$ versus $\ln(B)$ and $\ln(Y)$ versus $\ln(C)$. Only correlation coefficients close to one should be included in the relationship equations.

The multiple linear regression analysis, with different combinations (ABC, ABD, ABE, ABF, ABG, BCD, BCE, BC, etc.) and the $N1$, $N2$, and $N3$ values obtained after solving the different equations, illustrates the influence of these individual parameters $N1$, $N2$, and $N3$ on the Y values. For example, if certain $N1$ or $N2$ or $N3$ values are negative, then they have no effect on Y. Further, a comparison of the numerical values of $N1$, $N2$, and $N3$ will highlight the relative influences from each variable on the Y values.

In the present experimental work, the compressive strength values were taken as dependent parameters (Y), while the molar ratios of Al/Si, Ca/Si, and Ca/(Si + Al) were taken as independent parameters (namely, $A1$, $A2$, and $A3$).

It is assumed that the power term associated with each reacting species (Al/Si, Ca/Si, and Ca/(Si + Al)) is related to the gel formation and thereby the strength of the samples (indicated in numerical values of power $N1$, $N2$, and $N3$). Also, a numerical value close to 1 is considered as optimum correlation. In actual practice, correlation coefficient calculations among each of the above-mentioned individual combinations with compressive strength should provide values higher than 0.95.

Determination of the Moles of Al/Si, Ca/Si, and Ca/(Si + Al) from the Chemical Compositions. It is pertinent to recognize that silica (SiO_2), alumina (Al_2O_3), and calcia (CaO) mainly participated in the formation of Al-Si gel, Ca-Si gel, and Ca-Si-Al gel, all of which contributed to the compressive strength of the final product.

2. Materials (Details of the Materials)

The chemical compositions of fly ash and GGBS slag are given in Table 2.

The XRD pattern and SEM images of the samples are given below (Figures 1–4).

2.1. Alkaline Solution. The alkaline activator was a combination of sodium hydroxide and sodium silicate solutions, where sodium hydroxide solution (of 98% purity) was used as alkaline activator along with sodium silicate ($\text{SiO}_2 = 31.0\%$, $\text{Na}_2\text{O} = 11.6\%$, and water = 57.4%). These sodium hydroxide solutions of required molarity (6 M = 240 gm and 12 M = 480 gm) were separately prepared. Sodium hydroxide solution of the required molarity and the sodium silicate in liquid state were then mixed and stored at room temperature before use.

2.2. Sample Preparation for Experimental Study. Fly ash and GGBS, with 10% variation by weight in dry condition, were pan-mixed. The mixture varied from 80% fly ash and 20% GGBS (F80G20) to 30% fly ash and 70% GGBS (F30G70) in six different compositions (A to F). The mixtures were activated by adding alkaline activator solutions (6 M and 12 M sodium hydroxide separately) and sodium silicate solution and thoroughly mixed.

The external source materials (fly ash and GGBS) were mixed in proportions as described above. Depending on the mix proportion, the alkali activator solution quantities were varied. The minimum addition of solution was for the higher fly ash-based compositions, while the maximum was for the higher GGBS-based compositions. The fresh mixtures of six different compositions (with 6 M sodium hydroxide molarity) and six other different compositions (with 12 M sodium hydroxide molarity) were cast in 50 mm × 50 mm × 50 mm steel moulds. On completion of 7 days and 28 days of curing, the cubes were tested for compressive strength as per standard testing methods, under exposure to ambient conditions (temperature 25°C to 27°C and humidity 65% to 70%). The resultant empirical model has been based on the experimental results of approximately 500 test samples.

3. Results

Considering the molar quantities of each of the chemicals present in the individual compounds, Table 3 summarizes the details of Al/Si, Ca/Si, and Ca/(Si + Al) mole in each individual batch compositions along with the compressive strengths.

The correlation coefficient between experimental compressive strength (Y) and the individual values of $\ln$, Al/Si ratio, $\ln$, Ca/Si ratio, and $\ln$, Ca/(Si + Al) ratio for 6 M and 12 M samples are given in Figures 5–7.

TABLE 1: Dependent and independent variables.

Sample names	Y (dependent variable)	A (independent variable)	B (independent variable)	C (independent variable)
A	Y1	A1	B1	C1
B	Y2	A2	B2	C2
C	Y3	A3	B3	C3
D	Y4	A4	B4	C4
E	Y6	A5	B5	C5
F	Y6	A6	B6	C6

TABLE 2: Chemical analysis of fly ash and GGBS (in weight %).

Material	SiO ₂	Al ₂ O ₃	CaO	MgO	MnO ₂	TiO ₂	Iron oxide	LOI
Fly ash	60.8	26.34	1.17	1.31	—	—	4.21	1.8
GGBS	34.79	20.07	32.78	7.23	—	—	0.87	0.1

3.1. Intercept (K Value) Determination. Table 4 highlights the regression equations of the different experimental samples.

3.2. Multiple Linear Regression Analysis. It is observed that the correlation coefficient values for the different compositions are all nearly one and therefore multiple linear regression analysis was performed with all the different combinations with three different variables N1, N2, and N3. Figures 8–13 display the plots of N1, N2, and N3 with different combinations for 28 days of curing.

Table 5 brings out the trend of silica, alumina, and calcia moles and the ratios of Al/Si, Ca/Si, and Ca/(Si + Al) in the four combinations considered.

4. Analysis and Discussion

4.1. Analysis of N1 Values Both with Increasing Molarity of Alkaline Solution and with Increasing Compositions from A to F. Figures 8 and 9 corroborate N1 (related to Al/Si composition) variations with both increasing molarity and increasing compositions for 28 days of curing. However, with regard to the composition dependence, it is noticed (Figure 9) that the compositions 2(B + C + D) and 3(C + D + E) are critical as there is a fall in N1 values (representing fall in strength). The average chemical compositions were SiO₂ (0.7–0.8 mol), Al₂O₃ (0.23 mol), and CaO (0.27–0.33 mol). It may therefore be reasonable to conclude that a change in mechanism of strength development of the cubes occurred around this composition. This is found to be true for both 7 days' and 28 days' curing periods.

4.2. Analysis of N2 Values Both with Increasing Molarity of Alkaline Solution and with Increasing Compositions from A to F. Values of N2 (related to strength development by Ca/Si ratios) exhibited a general negative trend with regard to both the increasing molarity and the increasing compositions. The negative values indicated that they played no role in the strength development process. Here also it is noted that the middle compositions have shown negative values with regard to both the increasing molarity and the increasing combinations of compositions (compositions 2 and 3).

4.3. Analysis of N3 Values Both with Increasing Molarity of Alkaline Solution and with Increasing Compositions from A to F. Figure 12 shows the distribution of N3 values of Ca/(Al + Si) ratio with respect to the strength under increasing molarity of alkaline solution. It is shown that the middle compositions (comp. B and C) demonstrate positive trend with regard to strength for both 7 days' and 28 days' curing. These compositions, in fact, exhibited negative N2 values. It is deduced that the loss in strength in these compositions due to negative N2 values is compensated by positive N3 values. Also, compositions 1 and 4 show negative values indicating that N3 values in these compositions have played no role in strength development. Figure 13 shows the effect of composition on strength at different molarities. It is again observed that the middle compositions showed positive N3 values, while compositions 1 and 4 showed negative values in both low molarity and high molarity and also with increasing curing period. The composition where such strength changeovers in the mechanism have occurred was not unique and was dependent on many other factors such as activity of the reacting source materials which vary depending on their place of origin.

It may be noted that combinations 2 and 3 exhibited wide variations in relationship between compressive strength and N1, N2, and N3 values in the different samples. This could be interpreted as indirect evidence of the formation of transient Ca-Si based combinations and/or Ca-Al based combinations or some other unknown transient phase formations as reported by Pulgalia and Mondal [11] influencing compressive strength. While combinations 1 and 4 exhibited variations in mean and standard deviations of different experimental parameters (within acceptable 3%–5% variations), combinations 2 and 3 represented variations beyond 5%. However, the nature of the qualitative relationships as represented by variations in compositions with variations in compressive strength has suggested that the analytical results can be satisfactorily explained with the help of statistical tools like correlation coefficients and multiple linear regression analysis.

5. Summary

The study conducted several experiments to determine the alkali concentration in a fly ash-GGBS geopolymer combination with varied molar concentrations of 6 mol to 12 mol with increments of two mol in six different fly ash-GGBS combinations with a minimum of 20 percent and a maximum of 70 percent GGBS. Multiple linear regression analysis with compressive strength (as dependent

FIGURE 1: XRD pattern of fly ash.

FIGURE 2: XRD pattern of GGBS.

FIGURE 3: SEM image of fly ash.

FIGURE 4: SEM image of GGBS.

TABLE 3: The details of Al/Si, Ca/Si, and Ca/(Si + Al) moles in each individual batch compositions and their compressive strengths.

Composition fly ash-GGBS (F-G)	Ln (Al/ Si)	Ln (Ca/ Si)	Ln (Ca/ (Si + Al))	Ln comp. strength 7 days/(6 M) REVISED	Ln comp. strength 28 days/(6 M) REVISED	Ln comp. strength 7 days/(8 M) REVISED	Ln comp. strength 28 days/(8 M) REVISED	Ln comp. strength 7 days/ (10 M) REVISED	Ln comp. strength 28 days/ (10 M) REVISED	Ln comp. strength 7 days/ (12 M) REVISED	Ln comp. strength 28 days/(8 M) REVISED	Ln comp. strength 7 days/(10 M) REVISED	Ln comp. strength 28 days/(10 M) REVISED
80F/20G (A)	-1.30/	-1.63	-1.87	-27.66	-24.97	-28.14	-23.31	-27.8	-22.46	-23.23	-19.6	-23.31	-27.8
70F/30G (B)	-1.27/	-1.37	-1.62	-27.59	-24.88	-28.07	-23.11	-27.74	-22.31	-23.09	-19.32	-23.11	-27.74
60F/40G (C)	-1.24/	-1.08	-1.35	-27.1	-24.56	-27.57	-22.86	-27.26	-21.95	-22.91	-19.25	-22.86	-27.26
50F/50G (D)	-1.23/	-0.87	-1.14	-26.76	-24.15	-27.28	-22.62	-27.03	-21.89	-22.78	-19.21	-22.62	-27.03
40F/60G (E)	-1.20/	-0.65	-0.94	-26.58	-24.05	-27.05	-22.52	-26.74	-21.79	-22.50	-19.13	-22.52	-26.74
30F/70G (F)	-1.17/	-0.49	-0.77	-26.4	-23.96	-26.84	-22.37	-26.53	-21.58	-22.27	-18.87	-22.37	-26.53

FIGURE 5: Correlation coefficient between experimental compressive strength and Ln, Al/Si ratio for 6 M and 12 M samples.

FIGURE 6: Correlation coefficient between experimental compressive strength and Ln, Ca/Si ratio for 6 M and 12 M samples.

parameter) and individual values of Al/Si, Ca/Si, and Ca/(Si + Al))ratios (as independent parameters) was performed. The study demonstrated that the strength of a geopolymers was dependent on gel formation from Al/Si ratio, Ca/Si ratio, and Ca/(Si + Al) ratio and brought out the role played in the setting process during curing.

6. Prospects, Challenges, Future Work, and Limitations

The industrial wastes are being produced in large quantities globally with no effective disposal solutions. In this context, the study has attempted to explain the role of fly ash and

FIGURE 7: Correlation coefficient between experimental compressive strength and Ln, Ca/(Si + Al) ratio for 6 M and 12 M samples.

TABLE 4: Determination of K values from the linear regression equations.

Description of 6 mol samples	Linear regression equation	Numerical value of K to be subtracted from experimental compressive strength values
Al/Si, corr. coeff. = 0.95 (6 M, 7 days' strength)	$y = 18.84 + 10.86x$	
Ca/Si, corr. coeff. = 0.99 (6 M, 7 days' strength)	$y = 6.58 + 1.10x$	$18.84 + 6.58 + 7.02 = 32.44$
Ca/(Si + Al), corr. coeff. = 0.98 (6 M, 7 days' strength)	$y = 7.02 + 1.25x$	
Al/Si, corr. coeff. = 0.93 (6 M, 28 days' strength)	$y = 16.54 + 8.83x$	
Ca/Si, corr. coeff. = 0.98 (6 M, 28 days' strength)	$y = 6.57 + 0.90x$	$16.54 + 6.57 + 6.95 = 30.06$
Ca/(Si + Al), corr. coeff. = 0.98 (6 M, 28 days' strength)	$y = 6.95 + 1.03x$	
8 mol samples		
Al/Si, corr. coeff. = 0.97 (8 M, 7 days' strength)	$y = 19.18 + 11.11x$	
Ca/Si, corr. coeff. = 0.97 (8 M, 7 days' strength)	$y = 6.70 + 1.22x$	$19.18 + 6.70 + 7.09 = 32.97$
Ca/(Si + Al), corr. coeff. = 0.97 (8 M, 7 days' strength)	$y = 7.09 + 1.26x$	
Al/Si, corr. coeff. = 0.98 (8 M, 28 days' strength)	$y = 15.10 + 7.57x$	
Ca/Si, corr. coeff. = 0.88 (8 M, 28 days' strength)	$y = 6.59 + 0.83x$	$15.10 + 6.59 + 6.86 = 28.55$
Ca/(Si + Al), corr. coeff. = 0.95 (8 M, 28 days' strength)	$y = 6.86 + 0.86x$	
10 mol samples		

TABLE 4: Continued.

Description of 6 mol samples	Linear regression equation	Numerical value of K to be subtracted from experimental compressive strength values
Al/Si, corr. coeff. = 0.96 (8 M, 7 days' strength)	$y = 18.88 + 10.81x$	
Ca/Si, corr. coeff. = 0.97 (8 M, 7 days' strength)	$y = 6.73 + 1.17x$	$18.88 + 6.73 + 7.11 = 32.72$
Ca/(Si + Al), corr. coeff. = 0.95 (8 M, 7 days' strength)	$y = 7.11 + 1.22x$	
Al/Si, corr. coeff. = 0.96 (8 M, 28 days' strength)	$y = 14.39 + 6.91x$	
Ca/Si, corr. coeff. = 0.92 (8 M, 28 days' strength)	$y = 6.61 + 0.748x$	$14.39 + 6.61 + 6.85 = 27.85$
Ca/(Si + Al), corr. coeff. = 0.95 (8 M, 28 days' strength)	$y = 6.85 + 0.78x$	
12 mol samples		
Al/Si, corr. coeff. = 0.97 (12 M, 7 days' strength)	$y = 15.24 + 7.73x$	
Ca/Si, corr. coeff. = 0.97 (12 M, 7 days' strength)	$y = 6.46 + 0.74x$	$15.24 + 6.46 + 6.79 = 28.49$
Ca/(Si + Al), corr. coeff. = 0.97 (12 M, 7 days' strength)	$y = 6.79 + 0.86x$	
Al/Si, corr. coeff. = 0.98 (12 M, 28 days' strength)	$y = 12.10 + 4.95x$	
Ca/Si, corr. coeff. = 0.88 (12 M, 28 days' strength)	$y = 6.44 + 0.44x$	$12.10 + 6.44 + 6.67 = 25.21$
Ca/(Si + Al), corr. coeff. = 0.95 (12 M, 28 days' strength)	$y = 6.67 + 0.55x$

FIGURE 8: N1 values with increasing molarity (28 days' curing) combinations from A to F.

GGBS on compressive strength development by an empirical model. The major challenge for the researchers will be to find ways to increase the usage of these industrial wastes in proportion to their large production. The second challenge will be to accurately establish the individual/collective contributions of the waste constituents in the manufacture of construction materials without comprising on the

strength parameters. The scope of research work undertaken was limited to 6 M and 12 M. The study can be extended to cover 4 M, 8 M, and 14 M to validate the results of this study over a wider spectrum of research. Also, similar studies can be carried out on other industrial wastes such as metakaolin, silica fumes, slug, rice husk, and various mine wastes with different molarities.

FIGURE 9: N1 values with increasing composition (28 days' curing) combinations from A to F.

FIGURE 10: N2 values with increasing molarity of alkaline solution (28 days' curing).

FIGURE 11: N2 values with increasing composition combinations from A to F (28 days' curing).

FIGURE 12: N3 values with increasing molarity alkaline solution (28 days' curing) combinations.

FIGURE 13: N3 values with increasing composition from A to F (28 days' curing).

TABLE 5: Trend of silica, alumina, and calcia moles and the ratios of Al/Si, Ca/Si, and Ca/(Si + Al).

Combinations	SiO ₂ mol	Al ₂ O ₃ mol	CaO mol	Al/Si	Ca/Si	Ca/(Si + Al)
A + B + C (1)	0.87	0.24	0.22	0.28	0.25	0.20
B + C + D (2)	0.83	0.23	0.27	0.28	0.33	0.25
C + D + E (3)	0.78	0.23	0.33	0.29	0.42	0.32
D + E + F (4)	0.74	0.22	0.38	0.30	0.51	0.40

7. Conclusions

The proposed empirical model of the geopolymer reactions has drawn out the following conclusions:

- (1) Depending on overall silica, alumina, and calcia ratios in the mix compositions, the compressive

strength changed and this aspect was found to be dependent on overall Al/Si, Ca/Si, and Ca/(Si + Al) ratios.

- (2) The mix compositions (B and C) showed positive trend with regard to the compressive strength, for both 7 days' and 28 days' curing.

- (3) An interdependence between Ca/Si ratio and Ca/(Si + Al) ratios is found to exist. A fall in the strength due to Ca/Si ratio catalyzes the role of Ca/(Si + Al) to become more effective towards strength development of tested bricks.
- (4) The method proposed in the study, involving the combination of correlation coefficient and linear regression analysis, is considered useful to empirically capture the complex nature of geopolymerization.

Data Availability

The data used to support the findings of this study are included within the article, and further data or information required is available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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