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STATISTICAL OPTIMIZATION AND UNCERTAINTY ANALYSIS OF SUSTAINABLE GEOPOLYMER BINDER SYSTEMS USING TAGUCHI METHODOLOGY AND MONTE CARLO SIMULATION

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ABSTRACT

This study presents the parametric optimization of fly ash–GGBS based geopolymer paste using the Taguchi L25 orthogonal array combined with Monte Carlo Simulation (MCS) for performance prediction and reliability assessment. Four key parameters—fly ash content, GGBS percentage, NaOH molarity, and alkaline activator-to-binder ratio—were analyzed at five levels to evaluate their effect on compressive strength. The Taguchi method reduced the experimental trials from 625 to 25 specimens, while MCS assessed variability and reliability through statistical simulation. Experimental analysis using S/N ratio and ANOVA identified GGBS content and NaOH molarity as the most significant factors influencing strength. The optimum mix, consisting of 60% fly ash, 40% GGBS, 12M NaOH, A/B ratio of 0.3, and SS/SH ratio of 2, achieved an average compressive strength of 45.32 MPa. Monte Carlo results confirmed high reliability and low variability, demonstrating that the combined Taguchi–MCS approach is effective for designing sustainable and high- performance geopolymer paste for construction applications.

KEYWORDS: Geopolymer Concrete, Fly ash, Taguchi, ANOVA, Mix Design, GGBS

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INTRODUCTION

The increasing demand for environmentally sustainable construction materials has intensified the search for alternatives to ordinary Portland cement (OPC), whose production contributes significantly to global CO_2 emissions. Geopolymer concrete (GPC), produced through the alkaline activation of aluminosilicate-rich industrial by-products such as fly ash and ground granulated blast furnace slag (GGBS), has emerged as a promising low-carbon substitute. In addition to its environmental benefits, GPC exhibits favorable mechanical properties, enhanced durability, and superior resistance to chemical attack. However, the performance of geopolymer concrete is highly sensitive to its mix composition, particularly the proportions of fly ash and GGBS, the concentration of alkaline activators, and the alkaline activator-to-binder (A/B) ratio. Therefore, optimizing these parameters is essential to achieve desired strength characteristics and consistent performance.

Traditional experimental approaches for mix design optimization often require extensive trial casting, making them time-consuming, costly, and material intensive. Statistical design techniques such as the Taguchi method provide an efficient alternative by minimizing the number of experiments while effectively capturing the influence of critical factors. The Taguchi orthogonal array approach enables systematic investigation of multiple parameters at different levels and facilitates the identification of optimal combinations that maximize mechanical performance. In addition to experimental optimization, probabilistic techniques such as Monte Carlo Simulation (MCS) have gained importance in evaluating variability and reliability in material performance. MCS uses repeated random sampling to predict strength distributions, assess uncertainty, and estimate the probability of achieving target performance under varying conditions, thereby improving confidence in optimized mix designs.

In this context, the present study focuses on the parametric optimization of fly ash–GGBS based geopolymer concrete using the Taguchi L25 orthogonal array integrated with Monte Carlo Simulation. Four major factors—fly ash content, GGBS percentage, NaOH molarity, and alkaline activator-to-binder ratio—were analyzed to determine their influence on compressive strength and identify the optimal mix combination with minimal experimental effort. Although several studies have investigated geopolymer concrete, there remains a significant research gap in achieving statistically validated optimum mix proportions with fewer experimental trials. This study addresses this gap by combining the efficiency of the Taguchi method with the predictive and reliability assessment capability of Monte Carlo Simulation. The findings contribute to the development of reliable, sustainable, and high- performance geopolymer concrete mixtures for modern construction applications.

EXPERIMENTAL METHODS:

Materials:

- Binders: Fly ash (FA) and GGBS were used as alumina silicate sources. Four levels of Flyash and GGBS replacement were considered: 20%, 40%, 60% and 80%.
- Alkaline Solutions: A combination of sodium hydroxide (NaOH) and sodium silicate solutions was used. NaOH molarity was varied at 6M, 8M, 10M, 12M, and 16M.
- Water: Distilled water was used for preparing NaOH solution

Fig. 1: Materials- Fly ash, NaOH pallets, Na2SiO3 solution and Potable water

Along with fly ash and GGBS as the primary pozzolanic binders, an alkaline activator solution consisting of sodium silicate (Na_2SiO_3) and sodium hydroxide (NaOH) pellets was used to initiate the geopolymerization process. The alkaline solution was prepared by dissolving sodium hydroxide pellets in distilled water to obtain the required molarity, after which sodium silicate solution was added and thoroughly mixed. The prepared solution was allowed to rest for approximately 24 hours prior to specimen casting to ensure stability. During mixing, the dry materials were first blended uniformly, followed by the gradual addition of the alkaline solution until a homogeneous and workable consistency was achieved. The fresh geopolymer concrete was then cast into cube molds and compacted using vibration. The specimens were cured under controlled conditions at 24°C and 20% relative humidity, demolded after 12 hours, and tested for compressive strength at 28 days.

Mix Design Preparation Using the Taguchi Method Orthogonal Array:

In parameter design experiments, the objective is to identify the optimal combination of input parameters that maximizes the desired quality characteristic while minimizing sensitivity to variations. When multiple factors are involved, the Taguchi method provides a systematic and efficient approach for determining the best parameter settings to achieve optimum performance. By employing orthogonal arrays, the Taguchi technique enables the study of several factors simultaneously with a significantly reduced number of experiments, thereby minimizing time, cost, and material consumption. Furthermore, the results obtained from a limited set of experiments can be effectively extended over a broader experimental range.

The experimental results were analyzed using Analysis of Variance (ANOVA) to evaluate the contribution of each independent variable to the compressive strength of geopolymer concrete (GPC). ANOVA is a statistical tool used to quantify the relative influence of each factor on the response by expressing its contribution as a percentage of the total variation. This is determined from the ratio of the sum of squares of each factor to the total sum of squares. In addition to ANOVA, Monte Carlo Simulation (MCS) was employed to assess the variability and reliability of the compressive strength predictions. MCS uses repeated random sampling to generate strength distributions under varying input conditions, allowing the estimation of uncertainty and the probability of achieving target performance levels. This probabilistic analysis enhances the reliability of the optimization process and validates the consistency of the predicted results.

In this study, an L25 orthogonal array was selected for the experimental design, allowing the evaluation of four factors at five levels each, thereby reducing the total number of possible combinations from 625 (5^4) to only 25 experimental trials. The selected factors and their corresponding levels are as follows:

Table 1: The Factors Details for Mix Design

Factor	Level 1	Level 2	Level 3	Level 4	Level 5
GGBS Replacement (%)	0	10	20	30	40
AS/B Ratio	0.3	0.4	0.5	0.6	0.7
NaOH Molarity (M)	6	8	10	12	16
Activator Ratio	1	1.5	2	2.5	3

The following are the output for Taguchi orthogonal array combinations from the MINITAB software are as follows. For each experimental trial, the geopolymer mix was prepared according to the proportions specified in the above table and cast into cube specimens of size 70.6 × 70.6 × 70.6mm. The specimens were then cured under ambient conditions for 28 days. After the curing period, compressive strength testing was conducted in accordance with the procedures specified in IS 516: 1959

Table 2: Taguchi Orthogonal Array combination from Minitab Software

Sl. No.	Molarity	GGBS%	SS/SH Ratio	Alkaline/ Binder Ratio
1	6	0	1	0.3
2	6	10	1.5	0.4
3	6	20	2	0.5
4	6	30	2.5	0.6
5	6	40	3	0.7
6	8	0	1.5	0.5
7	8	10	2	0.6
8	8	20	2.5	0.7
9	8	30	3	0.3
10	8	40	1	0.4
11	10	0	2	0.7
12	10	10	2.5	0.3
13	10	20	3	0.4
14	10	30	1	0.5
15	10	40	1.5	0.6
16	12	0	2.5	0.4
17	12	10	3	0.5
18	12	20	1	0.6
19	12	30	1.5	0.7
20	12	40	2	0.3
21	14	0	3	0.6
22	14	10	1	0.7
23	14	20	1.5	0.3
24	14	30	2	0.4
25	14	40	2.5	0.5

Mixing Combination, Mixing Procedure:

The NaOH solution was prepared 24 hours before mixing to allow the heat generated during the reaction to stabilize. Sodium silicate was then added 5 hours before casting to obtain a uniform alkaline solution. First, the dry materials were mixed thoroughly, and then the alkaline solution was added gradually. Mixing was continued until a uniform and workable mix was obtained. The fresh concrete was poured into cube molds and compacted using vibration. The specimens were cured at 24°C and 20% relative humidity, demolded after 12 hours, and tested for compressive strength after 28 days.

Fig. 2: Casting and Curing Process

Testing Methodology:

A compressive strength test was employed on 70 .6mm cubes using the 300 T capacity of a compression testing machine supplied by Aimil Ltd., Delhi, India. Three specimens were cast for each mixture and tested according to IS 516. The compression testing machine used in this study is shown in following Figure.

Fig. 3: Testing of Specimen in Compression Testing Machine

RESULTS AND DISCUSSION:

Table shows the Taguchi model used to determine the optimum compressive strength of geopolymer concrete (GPC) and the corresponding parameter combinations. For each experimental trial, three specimens were cast and tested under compression, and the average value was considered as the compressive strength, as commonly followed in concrete research. If any individual result deviated by more than 10% from the mean value, it was discarded and a new set of specimens was prepared to ensure result accuracy. The effect of each parameter on compressive strength development is illustrated in Figure, which was obtained by analyzing the experimental data presented in the table.

Table 4: Average Compressive Strength

Tr. No.	Molarity	Average Strength (kN/mm2)		
T1		58.92	90.76	104.63
T2		76.81	103.21	119.32
T3	6	82.31	94.72	109.12
T4		83.91	93.24	127.62
T5		92.12	99.17	129.62
T6		81.32	98.34	139.21
T7		80.73	87.43	106.12
T8	8	74.24	78.78	109.13
T9		79.90	83.91	123.13
T10		110.21	129.22	161.24
T11		89.30	101.82	113.72
T12		92.41	99.83	107.28
T13	10	99.38	103.43	121.42
T14		101.24	113.97	126.42
T15		119.33	123.54	134.32
T16		145.31	153.24	173.76
T17		120.28	130.93	144.73
T18	12	150.38	163.24	179.48
T19		140.13	151.43	169.54
T20		190.24	203.48	224.39
T21		45.24	58.24	69.34
T22		80.61	92.16	108.72
T23	14	85.94	98.77	112.72
T24		90.23	101.34	127.85
T25		80.19	97.64	131.44

In addition, Monte Carlo Simulation (MCS) was performed to assess the variability and reliability of the compressive strength results by generating repeated random samples and predicting strength distributions. The simulation confirmed the consistency of the experimental findings and validated the optimized mix performance. Among all the mixes, Mix M20 achieved the highest average compressive strength of 224.39 kN (45.32 MPa), corresponding to the optimum parameter combination of 40% GGBS, activator-to-binder ratio of 0.3, NaOH molarity of 12M, and activator ratio of 2.0.

Taguchi Analysis: Influence of Parameters on Compressive Strength

The Taguchi method allows for evaluating multiple factors systematically using a minimal set of experiments. In this study, the compressive strength of each mix (M1 to M25) was evaluated using the "larger-the-better" quality characteristic, which emphasizes maximizing strength. Signal-to-noise (S/N) ratios were calculated for each trial using:

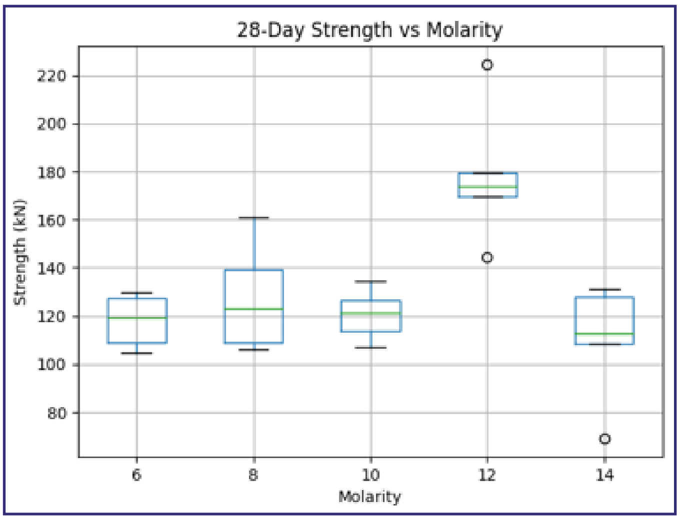
$$\text{S/N Ratio (Larger is Better)} = -10 \cdot \log_{10}\left(\frac{1}{n}\sum_{i=1}^{n}\frac{1}{y_i^2}\right)$$

The ANOVA results indicate that molarity has a statistically significant influence on the 28-day compressive strength of geopolymer concrete ($F = 8.426$, $p = 0.000373$). Since the p-value is less than 0.05, the null hypothesis is rejected, confirming that variations in NaOH molarity significantly affect strength development. The results further show that the 12M concentration produced the highest compressive strength, demonstrating its optimum effectiveness for geopolymerization, while excessive molarity (14M) resulted in strength reduction due to possible alkali saturation effects.

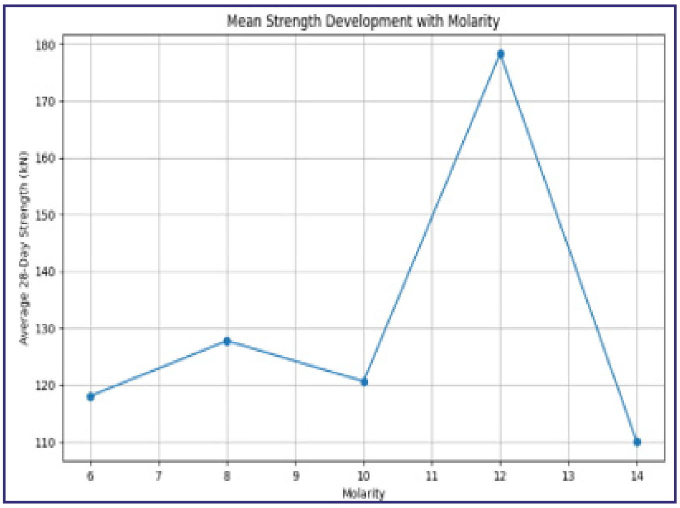
ANOVA Results (28-Day Strength vs Molarity)

- F-value: 8.426
- p-value: 0.000373

Since $p < 0.05$, molarity has a statistically significant effect on compressive strength. This confirms your experimental conclusion that NaOH molarity strongly influences geopolymer strength development, with 12M giving the optimum performance.



The box plot illustrates the distribution of 28-day compressive strength values for different NaOH molarities. It is evident that the 12M molarity exhibits the highest median compressive strength along with a relatively narrow interquartile range, indicating superior strength performance with good consistency. The 6M and 8M molarities show moderate strength values with noticeable variability, suggesting incomplete geopolymerization at lower alkaline concentrations. The 10M molarity demonstrates stable performance but does not achieve the peak strength observed at 12M. In contrast, 14M molarity shows a wider spread and lower median strength, indicating inconsistent performance likely caused by excessive alkalinity, which may hinder proper geopolymer matrix formation. Overall, the box plot confirms that 12M is the optimum molarity for achieving high and reliable compressive strength.



The mean plot presents the average 28-

day compressive strength variation with respect to NaOH molarity. The trend shows a steady increase in compressive strength from 6M to 12M, indicating improved geopolymerization and stronger binder matrix formation with increasing alkaline concentration. The maximum average strength is achieved at 12M, confirming it as the optimum molarity for the investigated mix proportions. Beyond this optimum level, a decline in strength is observed at 14M, which may be attributed to excess hydroxide ions causing rapid precipitation and incomplete polymer chain development. This trend clearly demonstrates that there exists an optimum molarity level beyond which the mechanical performance of geopolymer concrete decreases. The mean plot therefore validates the Taguchi optimization results and supports the reliability predictions obtained through Monte Carlo Simulation.

The histogram of Monte Carlo simulated 28-day compressive strength shows an approximately normal distribution around the mean value, indicating stable probabilistic behavior of the optimized geopolymer concrete mix. The concentration of most simulated values near the central region confirms low variability and high reliability of the mix design. The narrow spread of the histogram suggests consistency in strength development, validating the effectiveness of the Taguchi optimization approach combined with Monte Carlo Simulation for reliable compressive strength prediction.

CONCLUSION:

1. The Taguchi L25 orthogonal array integrated with Monte Carlo Simulation (MCS) successfully optimized the fly ash–GGBS based geopolymer concrete mix design with reduced experimental effort and improved statistical reliability.
2. The optimum mix proportion was identified AS 60% fly ash, 40% GGBS, activator-to-BINDER ratio of 0.3, Na_2SiO_3/NaOH ratio of 2, and 12M NaOH concentration.
3. The optimized mix (T20) achieved the highest 28-day compressive strength of 224.39 kN (45.32 MPa) under ambient curing conditions, indicating superior geopolymerization performance.
4. The Taguchi method reduced the total number of experimental combinations from 625 to only 25 trials, making the optimization process economical, efficient, and less time- consuming.
5. ANOVA results confirmed that NaOH molarity significantly influenced compressive strength development with an F-value of 8.426 and p-value of 0.000373, indicating strong statistical significance.
6. The mean plot showed that compressive strength increased steadily from 6M to 12M and decreased at 14M, confirming that 12M is the optimum alkaline concentration for maximum strength development.
7. The box plot analysis revealed that the 12M molarity exhibited the highest median strength with comparatively lower variability, indicating stable and consistent performance.
8. Monte Carlo Simulation validated the experimental results through repeated random sampling, confirming the high reliability, low variability, and consistency of the optimized mix.
9. The probabilistic assessment demonstrated that the optimized geopolymer mix is capable of maintaining dependable compressive strength performance under practical material variations and uncertainties.
10. The Monte Carlo simulation histogram exhibited an approximately normal distribution with a narrow spread around the mean strength, confirming the low variability, statistical consistency, and high reliability of the optimized geopolymer concrete mix design.
11. The combined Taguchi–Monte Carlo framework proved to be a robust and effective optimization technique for developing sustainable, high-performance geopolymer concrete suitable for structural applications.
12. The optimized fly ash–GGBS geopolymer concrete offers significant potential as an environmentally sustainable alternative to conventional OPC-based concrete.
13. Future studies may extend this work to evaluate durability, impact resistance, abrasion resistance, and long-term structural performance by incorporating additional influencing parameters for further optimization.

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