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MIX PROPORTION OF FLY ASH AND SILICA FUME MORTAR USING THE ANN-GRADIENT DESCENT MODEL FOR PREDICTING COMPRESSIVE STRENGTH

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ABSTRACT: This study develops an Artificial Neural Network with Gradient Descent (ANN-G) model to predict the compressive strength of geopolymer mortar based on fly ash and silica fume mix proportions. Accurate prediction of compressive strength is essential for optimizing geopolymer mixes and promoting sustainable construction practices. The research employs the Taguchi experimental design to optimize the geopolymer mix for target strengths of 30 MPa, 35 MPa, and 40 MPa. The ANN-G model predicts compressive strengths of 26.92 MPa, 35.15 MPa, and 40.35 MPa, demonstrating its accuracy and efficiency. Results show that the ANN-G model outperforms conventional ANN models by reducing prediction errors and improving reliability. This approach streamlines the mix design process, reduces the need for extensive experimental testing, and enhances prediction accuracy. The ANN-G model offers a practical tool for designing geopolymer mortars in construction. Future work should focus on integrating larger datasets and exploring hybrid models to improve prediction stability and extend the model's applicability in real-world construction scenarios.

Keywords: Artificial neural network, Gradient boosting, Taguchi experiment, Geopolymer mortar

1. INTRODUCTION

Geopolymer concrete serves as an alternative binding agent to reduce the use of ordinary Portland cement (OPC) in construction. It decreases energy consumption and CO_2 emissions as a binder [1]. Fly ash enhances concrete properties, particularly compressive strength [2]. Estimating compressive strength based on mix proportions provides significant benefits for construction and material design, accelerating the design and decision-making process for predicting the strength of concrete or geopolymer mixes [3]. Accurate prediction of compressive strength ensures efficient material usage, minimizes waste, and reduces overall project costs [4]. This approach helps achieve the desired strength while avoiding overdesign, which can lead to unnecessary expenses. Additionally, it supports sustainability by integrating alternative materials, maintaining performance, and reducing the environmental impact of construction [5].

A well-structured experimental design ensures reliable results by systematically covering all factor combinations, simplifying complex systems, and revealing variable interactions. It reduces experimental workload, lowers costs, and maintains statistical accuracy. Additionally, it optimizes processes by identifying key factors and supporting informed decision-making across various fields. The Taguchi method of experimental design efficiently analyzes complex variables using orthogonal arrays (OAs) to minimize experimental runs while ensuring statistical reliability [6, 7]. Each row in an OA represents a unique factor level combination, guiding experiments and measurements [8]. This method streamlines experimental design while providing robust results for systems with multiple variables and intricate interactions [9]. Developing predictive models based on experimental data offers numerous advantages, including enhanced accuracy and reduced reliance on trial-and-error experiments [10, 11]. These models enable the consistent achievement of desired properties such as compressive strength. They also provide insights into the influence of variables and activator concentrations, optimizing mix designs. Artificial Neural Networks (ANNs) are widely used for predicting geopolymer concrete strength [12, 13] due to their ability to model complex nonlinear relationships between inputs and outputs [14]. ANN reduces experimental workload and captures intricate variable interactions, making it essential for mix design optimization [15]. However, selecting the optimal number of nodes and hidden layers in an ANN is challenging, as it depends on problem complexity and input variables. Improper selection can lead to unfitting, reducing model performance [16].

Combining ANN with the gradient descent optimization algorithm provides an efficient solution by iteratively adjusting parameters to minimize errors between predicted and actual values [17]. This enables ANN to better learn complex patterns, making it a powerful tool for regression problems [18]. Gradient boosting further optimizes geopolymer mortar properties [19], allowing precise mix design optimization with minimal experimental effort. Its ability to capture complex relationships between input variables and target properties makes it valuable for advancing sustainable concrete technology [20]. When integrated with ANN, gradient boosting effectively handles noisy data, addresses feature interactions, refines predictions, and reduces errors, supporting sustainable construction by minimizing waste and promoting eco-friendly materials.

2. RESEARCH SIGNIFICANCE

The geopolymer mortar mix proportions derived from the developed contour plots were experimentally validated. The selected mixture requires balancing three input variables, and the proposed method effectively determines mix designs for fly ash and silica fume geopolymer mortar within the 30, 35, and 40 MPa range at 28 days. The experimental design was developed using the ANN-G regression model and the Taguchi method. This study demonstrates that ANN-G serves as an effective alternative to Taguchi, offering improved prediction accuracy and reliability. By reducing testing costs, this approach establishes robust regression models, paving the way for future studies to explore additional factors and advanced prediction techniques.

3. MATERIALS AND METHODS

Various mix design formulations were developed to synthesize fly ash and silica fume-based geopolymers, aiming to understand the effects of different component proportions on the properties of the resulting geopolymer mortars. Silica fume is commonly used in concrete to enhance its properties, particularly by increasing compressive strength [21]. Typically, silica fume (SF) replaces 20% of the total binder content [22, 23]. The composition of the binder material was analyzed using X-ray fluorescence (XRF) and is presented in Table 1.

Table 1. Chemical composition of Fly ash (FA) and Silica fume (SF) analyzed by XRF

Formula	Components	Fly ash (%)	Silica fume (%)
SiO_2	Silicon Dioxide	30.53	98.34
Al_2O_3	Aluminum Oxide	14.81	-
CaO	Calcium Oxide	21.08	0.25
SO_3	Sulfur Trioxide	7.22	0.14
Fe_2O_3	Iron (III) Oxide	14.4	0.04
Na_2O	Sodium Oxide	5.51	0.72

In this study, experimental binders were prepared with varying percentages of FA and SF. The binders contained 96%, 94%, and 92% FA, with the remaining portion replaced by 4%, 6%, and 8% SF, respectively. Alkaline activation solutions were used to assess their effects on the properties of geopolymer concrete. Sodium hydroxide (NaOH) solutions with molar concentrations of 6 M, 8 M, and 10 M were used, along with sodium silicate-to-sodium hydroxide (SS/SH) ratios of 1.0, 1.5, and 2.0. All mixes were activated with a constant liquid-to-solid (L/S) ratio of 1.0 and a fixed binder-to-sand ratio of 1:2.75 for all geopolymer mortar formulations.

3.1 Taguchi Experiment

The Taguchi experimental design is a systematic and efficient method for studying the effects of multiple variables on a process or product. It focuses on optimizing mix designs for concrete and geopolymer production. The Taguchi method employs an orthogonal array (OA) to minimize the number of experiments while ensuring an effective exploration of factor interactions. The key features are summarized in Table 2. In this study: A (%FA) represents the percentage of fly ash, while %SF denotes the percentage of silica fume in the binder mix. B (SS/SH) refers to the sodium silicate-to-sodium hydroxide ratio. C (Mol, M) indicates the molarity of sodium hydroxide (NaOH). The technical properties of various mix proportions were evaluated in the prediction process and verified through empirical correlations using mathematical equations derived from a limited experimental dataset.

The L9 Taguchi design method was used to predict compressive strength. NaOH powder was dissolved in water at concentrations of 6M, 8M, and 10M for 24 hours. NaOH and Na_2SiO_3 were then mixed, followed by the gradual addition of FA, SF, and river sand at low speed. The alkali-activated solution was blended and added to the dry ingredients, starting with 30 seconds of low-speed stirring, followed by 30 seconds at higher speed and scraping the pot sides. The mixture was then stirred at high speed for 60 seconds and poured into 50 mm cubic molds. The mortar specimens were cured in water for 28 days before testing. The mixing proportions of FA, SF, fine aggregates, and the alkaline activator are shown in Fig. 1.

Fig.1 Process of geopolymer mortar

Table 2. Mix design using the L9 orthogonal array

No.	Mix Design	A (%FA)	(%SF)	B (SS/SH)	C (Mol)	FA (g)	SF (g)	Fine Aggregate (g)	L/S Ratio	Na_2SiO_3 (g)	NaOH (g)
1	M1	96	4	1	6	710.4	29.6	2035	1	370	370
2	M2	96	4	1.5	8	710.4	29.6	2035	1	431.67	308.33
3	M3	96	4	2	10	710.4	29.6	2035	1	493.33	246.67
4	M4	94	6	1.5	6	695.6	44.4	2035	1	431.67	308.33
5	M5	94	6	2	8	695.6	44.4	2035	1	493.33	246.67
6	M6	94	6	1	10	695.6	44.4	2035	1	370	370
7	M7	92	8	2	6	680.8	59.2	2035	1	493.33	246.67
8	M8	92	8	1	8	680.8	59.2	2035	1	370	370
9	M9	92	8	1.5	10	680.8	59.2	2035	1	431.67	308.33

The influence of the three input variables on compressive strength was assessed. Regression analysis was conducted to examine the relationship between the inputs and the outputs.

The compressive strengths of the specimens at 28 days were used as a measure of their mechanical properties. Hybrid ANN-gradient boosting models were developed to calculate mix proportions for model validation. Three geopolymer concrete mix designs were prepared with targeted compressive strengths of 30, 35, and 40 MPa at 28 days.

3.2 Machine Learning

The present study utilized an ANN and a gradient descent algorithm to predict the compressive strength of mortar samples.

3.2.1 Artificial neural network

Artificial neural networks (ANNs) are a key application of machine learning for solving regression problems due to their ability to learn complex relationships between variables from training data. In this study, regression models were applied to predict the compressive strength of an alkali-activated solution based on FA and SF at various mix proportions. An ANN consists of three main layers: input, hidden, and output. This study developed an ANN with three hidden layers to evaluate the compressive strength of FA- and SF-based geopolymer mortars using experimental data. Each layer consists of interconnected nodes. A multi-layer perceptron (MLP) architecture was employed to enhance prediction accuracy and data processing. The MLP consists of multiple layers of neurons and utilizes backpropagation to optimize the network by adjusting weights and biases. This architecture enables the model to learn patterns from the training data and make accurate predictions. In an ANN, signals propagate forward, with each neuron computing a weighted sum of inputs, adding a bias, and applying an activation function to produce an output. The learning process minimizes prediction errors by comparing predicted and observed values through a cost function. Equation 1 defines the weight and bias updates.

$$f = \left(\sum_{i=1}^{n} x_i w_i + b \right) \quad (1)$$

where w_i is the weight, x_i is the input, b is the bias term, n is the number of inputs, and i is an index ranging from 1 to n.

3.2.2 Gradient boosting

Gradient boosting is a powerful ensemble method that enhances predictive accuracy and can be integrated with an ANN. It optimizes predictions by sequentially training weak models to correct the errors of previous iterations. This approach improves model accuracy by addressing specific weaknesses in ANN outputs and capturing complex feature interactions that the ANN might overlook, thereby enhancing overall prediction performance. The general form of the gradient boosting model is mathematically represented in Equation 2.

$$r_{im} = -\left[\frac{\partial L(y_{i,} F(x_i))}{\partial F(x_i)} \right]_{F(x)=Fm-1(x)} \quad (2)$$

where *L(y, F(x))* represents the loss function, typically based on the mean of the target variable. $F(X_i)$ is the prediction made by the previous model, with m to $m\text{-}1$ to indicate the prior iteration. m represents a weak learner, determined during training to minimize the loss function. x denotes the input features or data.

Fig. 3 illustrates a hybrid approach that combines ANN and gradient boosting techniques for predictive modeling in the context of compressive strength prediction. The process follows these steps:

- The three input variables—%FA (fly ash content), SS/SH (sodium silicate to sodium hydroxide ratio), and NaOH molarity—are recognized as critical factors affecting the compressive strength of mortar.

- The ANN processes the input data by computing a weighted sum of the inputs.
- The result of this sum is passed through a Rectified Linear Unit (ReLU) activation function, introducing non-linearity to model complex relationships in the data.
- The Stochastic Gradient Descent (SGD) backpropagation algorithm iteratively adjusts the weights and biases to minimize the error between predicted and actual outputs.
- The processed signals from the hidden layer produce the ANN output, representing an intermediate prediction.
- To refine this prediction, the gradient boosting technique is applied, which builds an ensemble of weak learners sequentially.
- The residual error from the ANN output is reduced step by step using these weak learners through gradient descent.
- This combined approach results in a highly accurate prediction of compressive strength.
- The hybrid model leverages ANN to capture non-linear patterns and gradient boosting to correct residual errors, enhancing overall predictive accuracy.

This hybrid methodology leverages the strengths of ANN and the residual error minimization of gradient descent to enhance predictive performance.

3.2.3 Parameter

The performance of an ANN model is influenced by its network architecture and parameter settings. The parameter values used in the neural network models are provided in Table 3. The gradient boosting model is constructed by correcting the errors made by the previous model. The parameters used in this experiment are listed in Table 4.

Table 3. ANN parameters

Model	ANN3
Hidden layer	2
Input	3
Neurons in the hidden layer	100,100
Learning rate	1
Output	1
Epochs	100
Loss	MSE

Table 4. Gradient boosting parameters

Parameter	Value
Max depth	8
Min samples split	5
Min samples leaf	5
Max features	3
Learning rate	1
Epoch	5

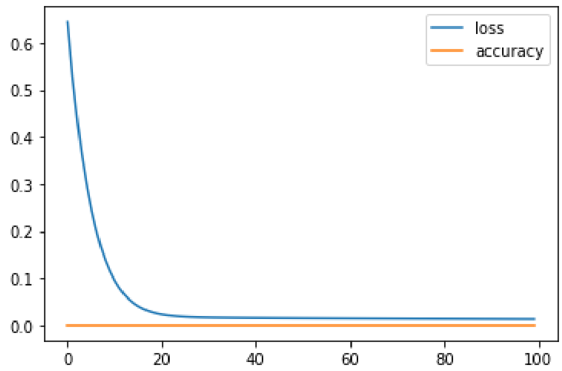

Fig 2. The loss versus the number of epochs for training data

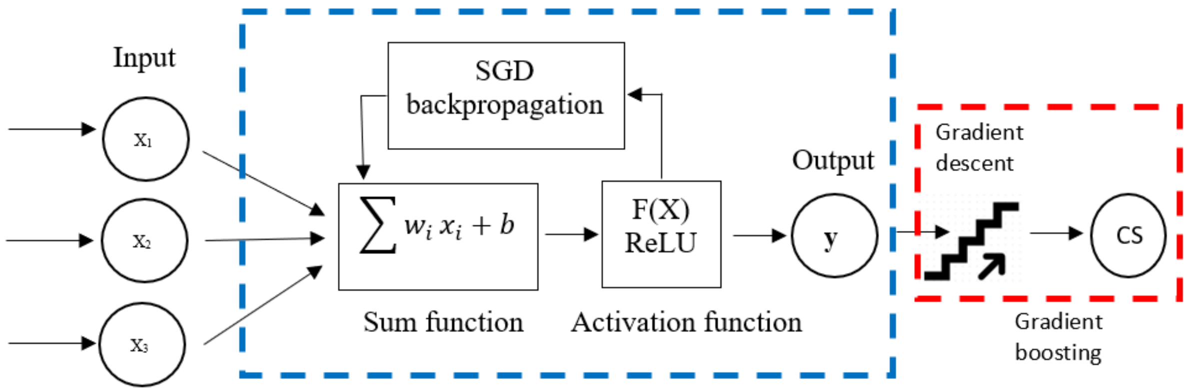

Fig.3 A fully connected artificial neural network and gradient boosting

Fig. 2 illustrates the relationship between the loss and the number of epochs during the training phase. As the number of epochs increases, the loss gradually decreases, indicating that the model is learning and improving its predictions over time. A stable and lower loss value towards the later epochs suggests that the training process is converging effectively.

3.2.4 K-Fold Cross-Validation for Model Performance Comparison

K-fold cross-validation is a resampling technique used to evaluate the performance of different models by splitting the dataset into K subsets (or folds), providing a more reliable assessment. This section presents the results of K-fold cross-validation for two models: ANN and ANN-G. The dataset was divided into 5 folds to represent the different subsets used in the cross-validation process.

Table 5. K-fold cross-validation

K-Fold	Model	Error Value 1	Error Value 2	Error Value 3
1	ANN	0.6316	-3.5444	2.7561
	ANN-G	0.7329	-3.4431	0.9851
2	ANN	2.6603	5.5313	3.6994
	ANN-G	2.4423	1.9035	2.2725
3	ANN	-0.4589	-4.6349	2.3637
	ANN-G	0.8368	-3.3392	0.7502
4	ANN	0.3383	-3.8377	3.6726
	ANN-G	0.7618	-3.4142	0.8258
5	ANN	8.5089	6.9998	6.4609
	ANN-G	1.6913	2.2056	1.6668

Table 5 shows that ANN-G generally yields lower errors in some instances, suggesting it may outperform ANN in specific scenarios. Additionally, random sampling plays a crucial role in model development, as fluctuations in the training data can impact prediction accuracy. To ensure the creation of a reliable predictive model, the experimental design must be carefully balanced and well-distributed.

4. RESULT AND DISCUSSION

The compressive strengths of the specimens at 28 days were used to assess their mechanical properties. For model validation, three geopolymer concrete mixes were designed with targeted compressive strengths (CS) of 30, 35, and 40 MPa at 28 days.

4.1 Mix Design of Geopolymer Mortar

The contour plots demonstrate the intercorrelation among the three selected inputs: the percentage of FA and SF, the Na2SiO3/NaOH ratio, and NaOH molarity, with the target output of compressive strength. These contour maps can therefore be used to design mix proportions for the target 28-day compressive strength of geopolymer mortar. Contour plots visualize how variables interact and influence the target compressive strength, helping to identify optimal parameter ranges for desired outcomes and making the design process more efficient. The color-coded zones make it easier to identify suitable combinations of input parameters to achieve specific target strengths, thus reducing the need for extensive trial-and-error experiments.

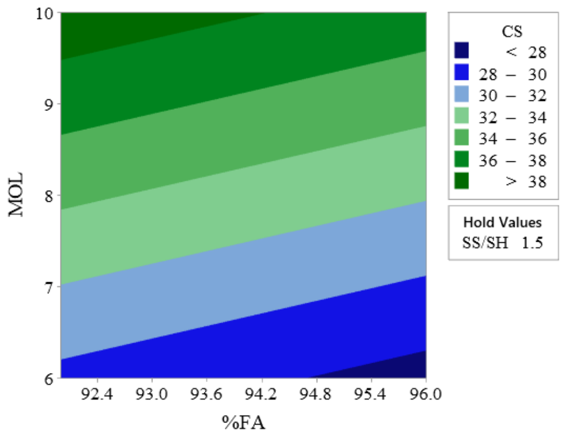

Fig 4. Contour plot showing the compressive strength

To determine the required values of %FA and MOL to achieve compressive strengths (CS) of 30, 35, and 40 MPa, the plot displays FA (Fly Ash) on the x-axis and MOL (Molarity) on the y-axis, with a constant SS/SH ratio of 1.5. The color gradients represent different ranges of compressive strength, as shown in Fig. 4. The regions corresponding to CS values of 30 MPa, 35 MPa, and 40 MPa are highlighted on the color-coded contour plot.

- For 30 MPa, the strength corresponds to the boundary between the blue and light green zones. The %FA range in this region is approximately 92 to 94, with MOL values between 6.0 and 6.5.
- For 35 MPa, the strength corresponds to the boundary between the light green and darker green zones. The %FA range is approximately 92 to 94, while the MOL values range from 8.0 to 8.5.
- For 40 MPa, the strength corresponds to the boundary near the transition from the darker green to the darkest green zone. The %FA range is approximately 92 to 94, with MOL values ranging from 9.5 to 10.0.

Table 6. Experiment from the contour plot

Target (MPa)	%FA	SS/SH	SH (M)	Exp	ANN	ANN-G
30	92	1.5	6	30.33	25.98	26.92
35	92	1.5	8	34.99	33.11	35.15
40	96	1.5	10	40.14	39.84	40.35

Table 6 shows the experimental results and predictions based on values derived from the contour plot. The comparison includes the target compressive strength, experimental results, and predictions using the ANN and ANN-G models. The parameters considered are %FA, SS/SH ratio, and NaOH molarity. The explanation is as follows:

• For a target compressive strength of 30 MPa, the experimental result was 30.33 MPa, closely matching the target. The mix parameters were %FA of 92, an SS/SH ratio of 1.5, and NaOH concentration of 6 M. The ANN and ANN-G models predicted compressive strengths of 25.98 and 26.92 MPa, respectively, slightly lower than the experimental value.

• For a target compressive strength of 35 MPa, the experimental result was 34.99 MPa, nearly identical to the target. The mix parameters were %FA of 92, an SS/SH ratio of 1.5, and NaOH concentration of 8 M. The ANN and ANN-G models predicted compressive strengths of 33.11 and 35.15 MPa, respectively, which were very close to the experimental result.

• For a target compressive strength of 40 MPa, the experimental result was 40.14 MPa, showing excellent consistency with the target. The mix parameters were %FA of 96, an SS/SH ratio of 1.5, and NaOH concentration of 10 M. The ANN and ANN-G models predicted compressive strengths of 39.84 MPa and 40.35 MPa, respectively, which closely matched the experimental value.

The experimental results closely match the target strengths, while the ANN predictions show good agreement with the experimental data. The ANN-G model demonstrates better prediction accuracy compared to the standard ANN model. ANN-G tends to align more closely with the experimental results, especially for higher target values. This suggests that the contour plot values and ANN-G predictions effectively guide mix design.

4.2 Data Analysis

4.2.1 Performance of the Predictive Model

Test data is crucial for evaluating the performance of a predictive model. To ensure that the prediction model provides reliable results, out-of-sample validation was conducted using entirely new data not included in the training data. This ensures the reliability and effectiveness of the evaluation by validating the model's accuracy and generalization on unseen data.

Table 7 provides specific mix designs along with the associated predicted values and errors for both the ANN and ANN-G models. The comparison between the ANN and ANN-G models for predicting compressive strength shows that ANN-G consistently yields more accurate results with smaller prediction errors. In most cases, ANN-G exhibits smaller errors than ANN, demonstrating better prediction accuracy. The ANN-G model shows superior prediction accuracy compared to the standard ANN model. However, both models exhibit small prediction errors relative to the experimental values.

Table 7. Comparison of compressive strength

Exp	% FA	M	SS/ SH	Prediction		Error	
(CS)	A	B	C	ANN	ANN-G	ANN	ANN-G
30.33	92	6	1.5	25.98	26.91	4.35	3.41
30.83	92	6	1.0	29.14	29.84	1.68	0.98
34.39	94	10	2.0	35.92	35.15	-1.53	-0.75
34.51	96	8	1.0	35.72	36.99	-1.22	-2.49
34.99	92	8	1.5	33.11	34.65	1.89	0.35
40.13	96	10	1.5	39.84	40.35	0.29	-0.22

4.2.3 Performance evaluation

The chart and data provided compare the performance of two models, ANN and ANN-G, in predicting the CS of mortar

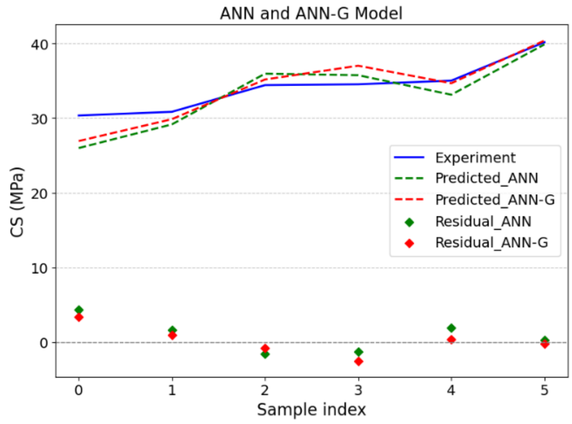

Fig 5. Multiple line and residual plots of predictions

Fig. 5 displays the actual measured values for each mix design. The blue line represents the experimental compressive strength, while the green dashed line shows the predictions made by the ANN model. Although the ANN predictions generally follow the experimental values, they exhibit larger deviations. In contrast, the red dashed line represents the predictions from the ANN-G model, which closely align with the blue line, indicating better accuracy and improved performance compared to the ANN model. ANN-G consistently shows smaller residual errors and aligns more closely with the experimental values, with its residuals tending to be closer to zero. This suggests a better fit to the experimental data. The gradient descent optimization in the ANN-G model improves its ability to find better weight values, leading to greater prediction accuracy. Overall, ANN-G proves to be a more reliable model for this application due to its higher precision and more favorable error distribution.

4.2.3 Normal distribution

The observed outcomes of the experiment are plotted against the theoretical quantiles of a normal distribution. The L9 Taguchi experimental design was used, with three samples for each run.

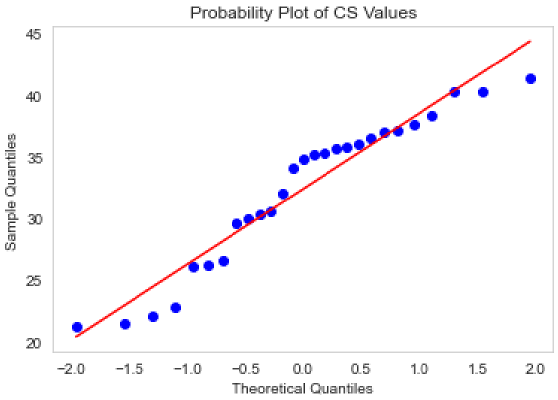

Fig 6. Probability plot for the L9 Taguchi experimental design

Fig. 6. The normal probability plot for the 9 data points from the Taguchi experiment shows that the blue points align closely with the red line, indicating that the data from the Taguchi experiment approximately follow a normal distribution.

4.2.4 Histogram

The histogram, with the aligned normal distribution curve, analyzes the distribution of data and represents the observed frequency of data values divided into intervals.

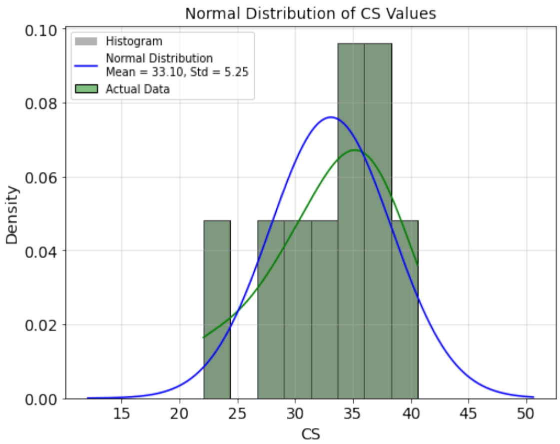

Fig 7. Normal distribution for the L9 Taguchi experimental design

A theoretical curve based on the mean (33.10) and standard deviation (5.25) of the data shows a well-distributed dataset, as seen in Fig. 7. The histogram aligns closely with the normal curve, suggesting the dataset is suitable for parametric analysis. However, the right-skewed distribution and the gap in CS values between 20 and 30 indicate low data density in this range, which may lead to prediction errors.

4.2.5 Relative importance of parameters

This highlights the significant contributions of three factors—%FA, SS/SH ratio, and molarity (Mol)—in influencing the compressive strength (CS).

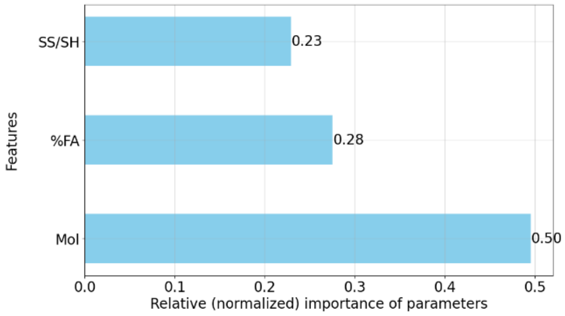

Fig 8. Relative importance of parameters influencing compressive strength

In the context of a Taguchi L9 design, Fig. 8 represents the calculated contribution of each parameter to the variation in CS. This analysis helps prioritize the parameters based on their influence. The molarity (Mol) parameter has the highest relative importance (50%), indicating its significant impact on CS. The percentage of fly ash (%FA) has moderate importance (28%), but its effect is less pronounced than that of Mol. The SS/SH ratio has the lowest relative importance (23%) and, consequently, the least impact on the response variable.

4.2.6 Main effect for compressive strength

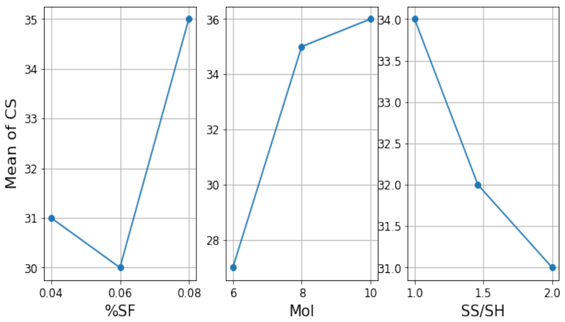

Fig 9. Main effect plot for compressive strength

Fig. 9. The main effect plot for compressive strength shows that increasing the percentage of silica fume (%SF) initially lowers the response but later enhances it. Molarity (Mol) strongly boosts CS, particularly between 6-8 M, with slower growth from 8-10 M. The SS/SH ratio negatively impacts CS, while higher NaOH concentration improves it. However, CS decreases as the Na_2SiO_3/NaOH ratio increases.

5. CONCLUSIONS

This study evaluates the use of ANN-G as an alternative to the Taguchi experimental design method. The results demonstrate that contour plots are a powerful tool for visualizing and estimating the compressive strength (CS) of geopolymer mortar before conducting experiments. These plots provide a solid foundation for mix design, enabling efficient parameter selection and reducing trial-and-error efforts, especially when combined with the predictive power of ANN-G.

• The experimental results closely align with the target compressive strengths, indicating an effective mix design. The ANN-G predictions show good accuracy at 35 MPa and 40 MPa, although there is a slight underestimation at 30 MPa.

• ANN-G outperforms ANN in terms of smaller errors and better residual distribution. The gradient descent optimization improves the model's predictive capacity, making ANN-G a more reliable choice for this application.

• The observed values are consistent with a normal distribution. Any small deviations from the line indicate slight randomness or experimental error, but they do not significantly affect the assumption of normality.

• The histogram curve reveals a well-distributed dataset, which is suitable for further statistical analysis and modeling that assumes data normality.

• The molarity (Mol) parameter has the highest impact on CS in this experiment, with a relative importance of 0.50.

This approach develops an ANN model with gradient descent to predict three target compressive strength levels: 30 MPa, 35 MPa, and 40 MPa. This combination enhances prediction accuracy while simplifying the development process, making it a practical choice for creating robust regression models for complex problems. ANN-G consistently outperforms ANN, demonstrating lower residual errors. Future work should consider incorporating other ensemble approaches, such as a hybrid ANN-SVM model, and testing the model on larger datasets to explore alternative optimization methods that could further minimize outliers and improve prediction stability.

6. ACKNOWLEDGMENTS

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