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Machine Learning Prediction of the 28-Day Compressive Strength of Ambient-Cured Geopolymer Concrete Using Ensemble Learning Algorithms

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ABSTRACT.
The nonlinear interactions among precursor composition, alkaline activator characteristics and mixture proportions complicate the prediction of compressive strength in geopolymer concrete. This study evaluated ensemble machine-learning algorithms for predicting the 28-day compressive strength of ambient-cured geopolymer concrete. Following data screening and removal of incomplete and duplicate observations, 251 mixtures were retained. Nine variables comprising fly ash, ground-granulated blast-furnace slag (GGBS), fine aggregate, coarse aggregate, NaOH, Na_2SiO_3, alkaline liquid-to-fly ash ratio, water-to-solids ratio and NaOH molarity were used as predictors. Random Forest, XGBoost, LightGBM, CatBoost and AdaBoost were evaluated using repeated five-fold cross-validation, with model performance assessed using the coefficient of determination (R^2), root mean square error (RMSE) and mean absolute error (MAE). Correlation analysis showed that GGBS exhibited the strongest positive linear association with compressive strength (r = 0.388), while fly ash showed a moderate negative association (r = −0.427). CatBoost achieved the highest predictive performance, with a mean cross-validation R^2 of 0.782 ± 0.100, RMSE of 8.13 ± 1.51 MPa and MAE of 5.37 ± 0.73 MPa, although XGBoost, LightGBM and Random Forest produced comparable performance. The results demonstrate that tree-based ensemble models can explain approximately 75–78% of the variation in 28-day compressive strength using routinely reported mixture and activator parameters. The models are best suited as preliminary screening tools within the represented mixture and ambient-curing domain rather than as substitutes for experimental validation.

Keywords: Geopolymer concrete, compressive strength, machine learning, CatBoost, ensemble learning, ambient curing, fly ash, GGBS

I. INTRODUCTION

Geopolymer concrete has attracted considerable attention as a lower-carbon alternative to Portland cement-based concrete because it can incorporate aluminosilicate-rich materials such as fly ash and ground-granulated blast-furnace slag (GGBS) [1]–[3]. Its compressive strength, however, depends on interacting factors including precursor proportions, alkaline activator composition, liquid content and curing conditions. These relationships are often nonlinear, which limits the reliability of simple empirical prediction methods across different mixture compositions [4]–[6]. Machine-learning techniques have therefore been increasingly applied to geopolymer-concrete strength prediction. Previous studies have employed artificial neural networks, Random Forest, AdaBoost, XGBoost and other ensemble approaches, with generally good predictive performance [4], [7], [8]. The novelty of current studies lies less in the use of machine learning itself and more in database quality, validation strategy and the robustness of the resulting models. However, predictive performance reported for geopolymer concrete varies considerably among studies because of differences in database composition, predictor selection, model optimisation and validation strategy. Performance estimates obtained from a single train–test partition may be sensitive to the specific observations assigned to each subset, especially for relatively small and heterogeneous datasets. Evaluation across repeated validation partitions is therefore useful for assessing the robustness and generalisation of competing models rather than relying solely on their best reported predictive accuracy.

Model performance is strongly influenced by the scope and structure of the database used for training. The database considered in the present study contains mixture-proportion and activator variables for geopolymer concrete tested at 28 days under ambient curing conditions of approximately 20–25 °C. The prediction problem was therefore restricted to the influence of mixture composition and alkaline activator characteristics on 28-day compressive strength. Nine input variables were considered: fly ash, GGBS, fine aggregate, coarse aggregate, NaOH, Na_2SiO_3, alkaline liquid-to-fly ash ratio, water-to-solids ratio and NaOH molarity.

Accordingly, this study compares Random Forest, XGBoost, LightGBM, CatBoost and AdaBoost for predicting the 28-day compressive strength of ambient-cured geopolymer concrete. Model performance was evaluated using repeated cross-validation together with R^2, RMSE and MAE. Emphasis was placed on comparative model robustness across validation subsets rather than on the highest accuracy obtained from a single data split. The resulting models are intended as preliminary screening tools for estimating compressive strength within the mixture domain represented by the database.

II. MATERIAL AND METHODS

A. Database development and screening

A database of geopolymer concrete mixtures was compiled from different experimental records from literature [2], [9]–[13]. The database initially comprised 254 observations containing information on precursor composition, aggregate content, alkaline activator characteristics, curing conditions and compressive strength. The principal variables included fly ash, ground-granulated blast-furnace slag (GGBS), fine aggregate, coarse aggregate, sodium hydroxide (NaOH), sodium silicate (Na_2SiO_3), activator liquid-to-fly ash ratio (AL/FA), water-to-solids ratio, NaOH molarity, curing age, curing temperature and compressive strength. The experimental database was screened prior to modelling to identify incomplete and duplicate observations. One record containing a missing water-to-solids ratio and one record without a reported compressive-strength value were excluded. One exact duplicate was also removed to prevent repeated weighting of an identical mixture, resulting in a final database of 251 unique and complete observations for model development.

Because all usable observations corresponded to a curing age of 28 days under ambient conditions (approximately 20–25 °C), curing age and curing temperature exhibited no meaningful variation and were consequently excluded as predictor variables.

B. Input and Output Variables

Following data screening, nine variables describing the geopolymer concrete mixture composition and alkaline activator characteristics were retained as model inputs. These comprised fly ash content, ground-granulated blast-furnace slag (GGBS) content, fine aggregate content, coarse aggregate content, sodium hydroxide (NaOH) content, sodium silicate (Na_2SiO_3) content, alkaline liquid-to-fly ash ratio (AL/FA), water-to-solids ratio and NaOH molarity. The 28-day compressive strength was selected as the continuous target variable. The input and output variables adopted for model development are summarised in Table 1.

TABLE I
INPUT AND OUTPUT VARIABLES USED FOR MACHINE LEARNING MODEL DEVELOPMENT

Variable	Abbreviation	Unit	Role
Fly ash	FA	kg/m^3	input
Ground-granulated blast-furnace slag	GGBS	kg/m^3	input
Fine aggregate	FAgg	kg/m^3	input
Coarse aggregate	CAgg	kg/m^3	input
Sodium hydroxide	NaOH	kg/m^3	input
Sodium silicate	Na_2SiO_3	kg/m^3	input
Alkaline liquid-to-fly ash ratio	AL/FA	-	input
Water-to-solids ratio	W/S	-	input
NaOH molarity	M	mol/L	input
Compressive strength	CS	MPa	output

C. Statistical and Correlation Analysis

Descriptive statistics, including the minimum, maximum, mean and standard deviation, were determined to characterise the distribution and range of the numerical variables. Pearson's correlation coefficient was subsequently used to examine pairwise linear associations between the input variables and compressive strength. Correlation analysis was used only as an exploratory tool and not as a basis for eliminating predictors, since weak linear correlation does not necessarily imply limited predictive importance in models capable of representing nonlinear relationships and interactions among variables [14]. The descriptive statistics obtained from the cleaned database are presented in Table 2.

TABLE II
DESCRIPTIVE STATISTICS OF THE GEOPOLYMER CONCRETE DATABASE

Variable	Minimum	Maximum	Mean	Standard deviation
Fly ash	0	523	175.78	170.61
GGBS	0	467	216.54	165.74
Fine aggregate	459	1332	733.09	122.99
Coarse aggregate	331	1298	1047.37	196.06
NaOH	3.50	147	63.82	30.50
Na_2SiO_3	22.60	234	106.97	30.38
AL/FA	0.10	0.84	0.425	0.081
Water/solids ratio	0.18	0.53	0.327	0.093
NaOH molarity	1	20	8.35	4.54
Compressive strength	8.00	81.24	41.20	18.02

Pearson's correlation coefficient was used as an exploratory measure of the linear association between the numerical input variables and compressive strength. The correlation coefficient r between variables X and Y was determined as:

$$r_{XY} = \frac{\sum_{i=1}^{n}(X_i - X)(Y_i - Y)}{\sqrt{\sum_{i=1}^{n}(X_i - \bar{X})^2}\sqrt{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}} \tag{1}$$

Where Xi and Yi represent individual observations while X¯and Y¯denote their respective means

The correlation analysis was employed principally for exploratory purposes and not as a basis for predictor elimination because Pearson's coefficient quantifies linear association, whereas the machine-learning algorithms considered in this study can represent nonlinear relationships and interactions among mixture variables. Consequently, a low Pearson correlation coefficient would not necessarily indicate that a predictor has little importance in the resulting nonlinear prediction model.

D. Machine-Learning Models

Five tree-based ensemble regression algorithms were evaluated: Random Forest (RF), Extreme Gradient Boosting (XGBoost), Light Gradient Boosting Machine (LightGBM), Categorical Boosting (CatBoost) and Adaptive Boosting (AdaBoost). Tree-based ensemble methods are particularly suitable for modelling complex nonlinear relationships and interactions among predictor variables and have been successfully applied to compressive-strength prediction in geopolymer systems [4], [6], [7].

Random Forest combines predictions from multiple decision trees generated using bootstrap samples and random subsets of predictor variables, thereby reducing the variance and overfitting associated with individual decision trees [15]. AdaBoost sequentially combines weak learners while placing increased emphasis on observations that are poorly predicted by preceding models [16]. XGBoost employs regularised gradient boosting to improve predictive performance while controlling model complexity [17], whereas LightGBM uses an efficient leaf-wise tree-growth strategy designed to improve computational performance [18]. CatBoost employs ordered boosting and symmetric decision trees to reduce prediction bias and improve model generalisation [19].

E. Model Development and Validation

The Model performance was evaluated using repeated five-fold cross-validation. In each cross-validation cycle, the database was divided into five subsets, with four subsets used for model training and the remaining subset used for validation. The procedure was repeated until each subset had served as the validation set. Five-fold cross-validation was repeated five times using different random partitions, resulting in 25 validation evaluations for each algorithm. A fixed random seed was used to ensure reproducibility of the data partitions.

F. Performance Evaluation

Model performance was evaluated using the coefficient of determination (R^2), root mean square error (RMSE) and mean absolute error (MAE), which are commonly employed for evaluating machine-learning regression models, including models developed for concrete and geopolymer strength prediction [4], [5], [7]. Higher R^2 values and lower RMSE and MAE values were considered indicative of better predictive performance. The coefficient of determination was calculated as:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{2}$$

Where y_i is the measured compressive strength, $\hat{y}_i$ is the model-predicted compressive strength and $\bar{y}$ represents the mean measured strength. An R^2 value approaching unity indicates that a larger proportion of the variability in compressive strength is explained by the model.

RMSE was determined from:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \tag{3}$$

While MAE was calculated as:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \quad (4)$$

RMSE assigns a relatively greater penalty to large prediction errors, whereas MAE represents the average absolute magnitude of the prediction errors. Consequently, models exhibiting higher R^2 together with lower RMSE and MAE were considered to provide superior predictive performance.

III. RESULTS AND DISCUSSION

A. Characteristics of the Geopolymer Concrete Database

The compressive strength of the 251 mixtures ranged from 8.00 to 81.24 MPa, with a mean of 41.20 MPa and standard deviation of 18.02 MPa, indicating that the database encompasses mixtures with substantially different strength levels.

Considerable variation was also observed in precursor composition. Fly ash content ranged from 0 to 523 kg/m^3, while GGBS varied from 0 to 467 kg/m^3. Consequently, the database included fly ash-dominant, blended fly ash–GGBS and GGBS-dominant formulations. Similar compositional diversity has been incorporated in previous ML studies of geopolymer concrete because variations in precursor proportions, alkaline activator characteristics and aggregate contents collectively influence strength development [4], [21].

The alkaline activator parameters also covered substantial ranges, with NaOH molarity extending from 1 to 20 M and AL/FA and W/S ratios ranging from 0.10–0.84 and 0.18–0.53, respectively. Previous studies have similarly identified activator concentration and activator-to-binder proportions as important parameters governing geopolymer-concrete strength [21].

Unlike the mixture variables, curing conditions exhibited essentially no variation in the available database. All usable observations corresponded to a testing age of 28 days under ambient curing conditions of approximately 20–25 °C.

B. Correlation Between Input Variables and Compressive Strength

Pearson correlation analysis revealed considerable differences in the magnitude and direction of the linear relationships between the input variables and compressive strength (Figure 1). GGBS exhibited the strongest positive correlation with compressive strength ($r \approx 0.39$), whereas fly ash showed a moderate negative correlation ($r \approx -0.43$). Fine aggregate exhibited a weaker positive relationship ($r \approx 0.28$), while Na_2SiO_3 showed a weak negative correlation ($r \approx -0.15$). The remaining variables exhibited relatively weak individual linear relationships with compressive strength.

The positive relationship between GGBS content and compressive strength is consistent with observations from previous data-driven studies of fly ash–slag geopolymer concrete. [21], using SHAP and partial-dependence analyses, found slag content to be among the most influential variables and reported a general increase in predicted compressive strength with increasing slag proportion. From a materials perspective, the contribution of GGBS can be associated with its calcium-rich composition and the development of calcium-containing reaction products alongside the aluminosilicate geopolymer network. However, the present correlation should not be interpreted as evidence that increasing GGBS content alone necessarily produces higher strength, because precursor proportions, activator composition and other mixture variables vary simultaneously within the database.

Similarly, the negative marginal correlation observed for fly ash does not imply that fly ash inherently reduces geopolymer-concrete strength. Fly ash and GGBS proportions vary considerably among the different mixture families, and an increase in one precursor may coincide with a reduction in the other. The observed coefficients therefore represent associations within the present multivariable database rather than isolated causal effects.

Interestingly, NaOH molarity exhibited only a weak marginal linear correlation with compressive strength in the present dataset. This contrasts with studies in which activator concentration emerged as an important predictor. [21], for example, identified molarity among the most influential variables and reported favourable strength behaviour around 14–16 M within their database, while a recent explainable-ML study also identified NaOH molarity as an important strength predictor. The difference reinforces the fact that a low Pearson coefficient does not necessarily indicate that molarity lacks predictive importance; its influence may be nonlinear and dependent on interactions with precursor composition and other activator parameters.

The generally modest pairwise correlations obtained for several variables demonstrate the limitations of describing geopolymer-concrete strength through isolated linear relationships. The coupled effects of precursor composition, activator characteristics and mixture proportions provide a rationale for the application of nonlinear machine-learning models capable of representing interactions among multiple predictors.

C. Comparative Performance of the Machine-Learning Models

The repeated cross-validation results are presented in TABLE and the comparative model performance in Figure 1. CatBoost achieved the highest mean predictive performance, with $R^2 = 0.782 \pm 0.100$, RMSE of 8.13 ± 1.51 MPa and MAE of 5.37 ± 0.73 MPa. XGBoost followed with $R^2 = 0.763 \pm 0.106$, while LightGBM and Random Forest produced similar mean R^2 values of 0.756 and 0.755, respectively. AdaBoost exhibited comparatively lower performance, with a mean R^2 of 0.666.

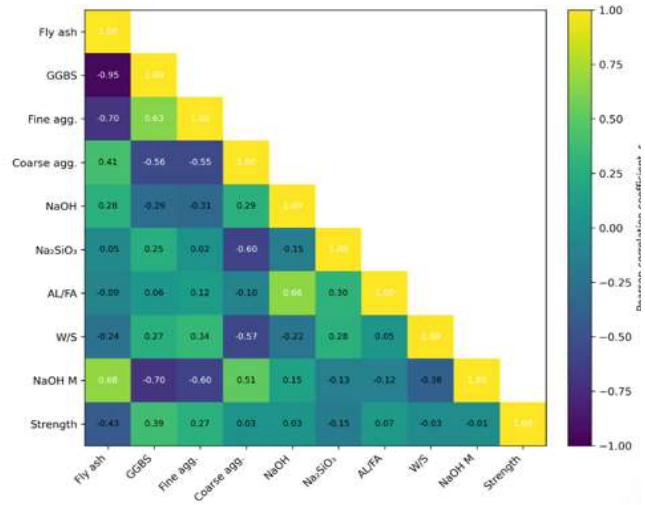

Figure. 1. Pearson correlation matrix of the input variables and compressive strength

The relatively strong performance of the tree-based ensemble algorithms is consistent with previous studies of geopolymer-concrete strength prediction. [4] demonstrated that ensemble-learning algorithms could effectively represent the nonlinear relationship between geopolymer mixture variables and compressive strength, while [6] similarly reported strong performance from ensemble-based models. A study of fly ash-based geopolymer concrete by [8] also demonstrated the effectiveness of ensemble artificial-intelligence approaches for strength prediction.

Particularly relevant to the present findings, [21], compared 11 machine-learning algorithms using 158 fly ash–slag geopolymer-concrete observations and repeated cross-validation. The four leading models were ranked CatBoost > XGBoost > Random Forest > Gradient Boosting, with CatBoost providing the best overall performance. This broadly agrees with the present results, in which CatBoost achieved the highest mean R^2, followed closely by XGBoost, with Random Forest also among the stronger models.

However, the differences among the four leading algorithms in the present study were relatively small. The difference between the mean R^2 values of CatBoost and XGBoost was only 0.019, while the corresponding differences relative to LightGBM and Random Forest were 0.026 and 0.027. These differences were smaller than the standard deviations observed across the repeated validation folds. CatBoost can therefore be identified as the highest-performing model under the adopted validation procedure, but the results do not establish overwhelming superiority over XGBoost, LightGBM or Random Forest.

D. Comparison with Predictive Performance Reported in Previous Studies

The predictive performance obtained in the present study is lower than some values reported previously for geopolymer-concrete strength prediction. For example, [6] reported an R^2 of approximately 0.97 for their best-performing bagging model, together with k-fold cross-validation. Other studies have likewise reported high predictive coefficients for machine-learning configurations.

Differences in reported predictive performance should be interpreted in relation to database size and heterogeneity, predictor selection, preprocessing procedures, model optimisation and validation strategy. The present analysis employed repeated cross-validation and reports mean performance across multiple validation partitions rather than relying on the performance obtained from a single train–test partition. Consequently, the mean R2 values obtained provide a more conservative estimate of expected performance across alternative subsets of the available database. Figure 3 shows a clear positive correspondence between measured and out-of-fold predicted compressive strengths, with most observations distributed around the line of perfect agreement. Greater dispersion is evident for some intermediate- and high-strength mixtures, indicating that prediction error is not uniform across the complete strength range. The pooled out-of-fold predictions yielded R2 = 0.783, RMSE = 8.39 MPa and MAE = 5.38 MPa, which are consistent with the mean repeated-cross-validation performance reported for CatBoost in Table 3.

TABLE III:
REPEATED CROSS-VALIDATION PERFORMANCE OF ENSEMBLE MODELS

Model	R^2	RMSE (MPa)	MAE (MPa)
CatBoost	0.782 ± 0.100	8.13 ± 1.51	5.37 ± 0.73
XGBoost	0.763 ± 0.106	8.48 ± 1.61	5.53 ± 0.83
LightGBM	0.756 ± 0.093	8.61 ± 1.43	5.64 ± 0.75
Random Forest	0.755 ± 0.111	8.61 ± 1.60	5.76 ± 0.90

AdaBoost	0.666 ± 0.098	10.18 ± 1.35	7.74 ± 0.79

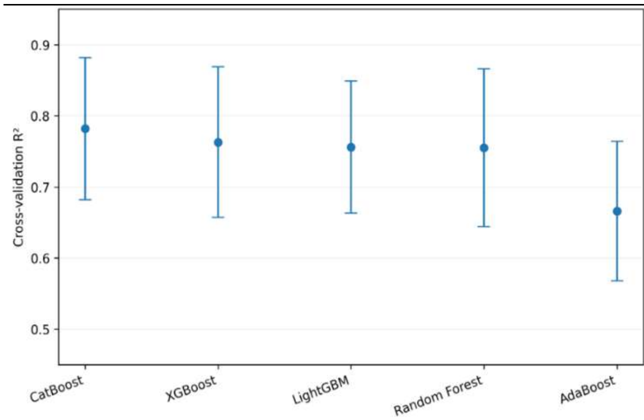

Figure 1: Mean R^2 and standard deviation of the ensemble models under repeated five-fold cross-validation.

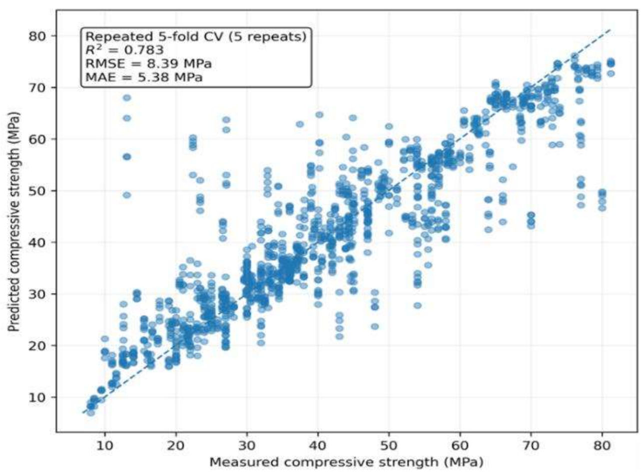

Figure 2: Measured versus predicted 28-day compressive strength using the CatBoost model

E. Prediction Error and Engineering Significance

The RMSE values of the four leading models ranged from approximately 8.13 to 8.61 MPa, while their MAE values ranged from 5.37 to 5.76 MPa. For CatBoost, the MAE of 5.37 MPa indicates that the predicted compressive strength differed from the measured value by approximately 5 MPa on average.

These errors should be considered relative to the broad compressive-strength range of the database (8.00–81.24 MPa). The results demonstrate that the models capture a substantial proportion of the overall strength variation but retain prediction errors that may be significant for individual mixture designs. The models should therefore be regarded as preliminary screening tools for estimating strength trends and identifying potentially promising mixtures rather than substitutes for experimental strength testing.

Previous ML studies similarly position predictive models as tools for supporting materials design and reducing the experimental search space rather than eliminating laboratory validation altogether [4], [7]. More recent work has extended this concept by integrating predictive models with optimisation frameworks for mixture selection.

F. Model Stability and Generalisation

The standard deviation of R^2 across repeated validation folds ranged from approximately 0.09 to 0.11 for the four leading models. This variability indicates that predictive performance was sensitive to the observations included in the training and validation subsets.

The result is important because the database contains only 251 observations and encompasses several distinct mixture families. Repeated cross-validation therefore provides additional information that would be lost if performance were reported only for a single train–test division. Repeated cross-validation has also been employed in previous fly ash–slag geopolymer-concrete ML research to provide a more robust assessment of model performance; [21], for example, used ten repeats of ten-fold cross-validation in comparing 11 algorithms.

G. Influence of Variables and Model Interpretation

The correlation analysis provides preliminary information regarding relationships between individual variables and compressive strength but cannot fully describe the nonlinear interactions represented by the ensemble models. Previous explainable-ML investigations have demonstrated that feature importance in geopolymer concrete can differ substantially from simple linear correlations [6], [21]. [21], for example, identified slag content, NaOH molarity, coarse aggregate, curing temperature and alkaline activator-to-binder ratio among the influential predictors in their fly ash–slag database. Recent explainable-ML work has similarly emphasised the importance of curing conditions, NaOH molarity, Si/Al ratio and precursor proportions.

The absence of precursor chemical composition, particle characteristics and variable curing conditions in the present database may therefore limit the extent to which the developed models can distinguish the physicochemical mechanisms responsible for strength development. Future databases incorporating such parameters would permit a more comprehensive interpretation of the relationships learned by the predictive models.

H. Limitations and Practical Implications

Despite the encouraging predictive performance, several limitations should be recognised. First, the final database contained 251 complete and unique observations, which is modest relative to the dimensionality and heterogeneity of the investigated mixture space. Second, source-study identifiers could not be recovered from the available project records, preventing study-level grouped validation. Third, the database contained mixture quantities and selected activator parameters but lacked detailed information on precursor chemistry, mineralogy, particle fineness and sodium silicate composition. Previous explainable-ML studies demonstrate that chemical and processing variables can contribute substantially to geopolymer strength prediction.

Finally, all usable observations represented 28-day strength under ambient curing. The resulting models should therefore not be extrapolated directly to other curing ages, elevated-temperature regimes or mixture compositions substantially outside the ranges represented in the database.

Within these constraints, the results demonstrate that ensemble-learning models can provide useful preliminary estimates of compressive strength from routinely reported mixture and activator parameters. Their principal application should be in screening candidate mixtures and supporting experimental planning, with final performance verified experimentally.

IV. CONCLUSION

This study investigated the application of machine-learning algorithms for predicting the 28-day compressive strength of ambient-cured geopolymer concrete using mixture composition and alkaline activator parameters. A database comprising 251 complete and unique observations was evaluated using five tree-based ensemble-learning algorithms, the principal findings are as follows:

i. The investigated database covered a broad compressive-strength range of 8.00–81.24 MPa and substantial variations in precursor, aggregate and alkaline activator characteristics, providing a heterogeneous basis for machine-learning model development.
ii. Pearson correlation analysis indicated that GGBS exhibited the strongest positive linear association with compressive strength ($r \approx 0.39$), while fly ash exhibited a moderate negative marginal correlation ($r \approx -0.43$). However, the generally weak correlations observed for several other variables highlight the limitations of pairwise linear relationships for describing the coupled effects governing geopolymer-concrete strength.
iii. CatBoost achieved the highest mean cross-validation performance (R^2=0.782 ± 0.100, RMSE = 8.13 ± 1.51 MPa and MAE = 5.37 ± 0.73 MPa), while XGBoost, LightGBM and Random Forest produced comparable performance. The relatively small differences among these models indicate that tree-based ensemble learning generally provided effective representation of the nonlinear relationships within the investigated database rather than demonstrating overwhelming superiority of a single algorithm. The observed variation in cross-validation performance demonstrates the importance of evaluating model robustness across multiple data partitions rather than relying solely on a single train–test split.
iv. The developed models are applicable primarily to the prediction of 28-day compressive strength under ambient curing and within the range of mixture characteristics represented in the database. Expansion of the database to include precursor physicochemical characteristics, additional curing regimes and independently sourced validation data would improve future model generalisation.

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