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ORIGINAL ARTICLE

Compressive strength prediction of sustainable concrete incorporating non-potable water via advanced machine learning

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Abstract: Concrete production imposes substantial environmental burdens, primarily through high carbon emissions and significant freshwater usage. This study addresses these challenges by developing a machine learning-based model to predict the compressive strength of concrete incorporating non-potable water, supporting sustainable construction practices. A comprehensive dataset of 1,056 samples was compiled from existing literature, encompassing key mix parameters such as fine and coarse aggregates, water-to-cement ratio, pH, and various supplementary cementitious materials. Multiple regression models were evaluated to predict compressive strength. Among these, the best-performing model achieved an R^2 of 0.98 and an RMSE of 1.45, demonstrating excellent predictive accuracy. Feature importance analysis identified the water-to-cement ratio, fine aggregate, and pH as the most influential variables affecting strength development. The study also applied explainable AI techniques to improve model interpretability and support informed engineering decisions. Sensitivity analysis confirmed model robustness across variable pH conditions, reinforcing its applicability to real-world wastewater variability. The results underscore the value of integrating non-potable water into concrete design and demonstrate the potential of optimized ML models to enhance resource efficiency, reduce environmental impact, and guide the development of greener infrastructure solutions.

Keywords: Non-potable water, sustainable concrete, compressive strength, LSBoost, machine learning.

1 Introduction

Concrete is among the most widely used construction materials globally, with its production projected to reach approximately 5.5 billion tons annually by 2050 [1]. While concrete offers notable structural benefits and versatility, its environmental drawbacks are substantial particularly in terms of carbon emissions and freshwater consumption. Cement manufacturing alone is responsible for approximately 5–8% of global CO_2 emissions due to its energy-intensive processes [2,3]. Furthermore, the high volume of freshwater required for concrete mixing exacerbates water scarcity, a pressing global issue affecting billions of people [4,5]. These environmental concerns underscore the urgency of developing sustainable alternatives, including the use of non-potable water sources in concrete

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production. To this end, various studies have examined alternative water sources such as treated wastewater, industrial effluents, and saline water for concrete mixing [6–8].

Concrete compressive strength prediction traditionally relies on two main approaches. The first involves mathematical and statistical modeling techniques, which depend heavily on the availability of large, high-quality datasets [9,10]. Although these models can yield accurate predictions under ideal conditions, their reliability diminishes with limited or noisy data. The second approach includes nonlinear forecasting models, which while flexible often lack a firm theoretical foundation and may only produce locally optimal results [11,12]. These limitations become particularly pronounced in complex environments, such as when concrete is exposed to aggressive chemical conditions like sulphate attack, where variable interactions are highly nonlinear and difficult to model using conventional techniques [13]. Artificial neural networks (ANNs), along with other machine learning (ML) techniques, have emerged as promising tools for modelling and predicting the mechanical performance of concrete materials in both conventional and harsh environmental conditions [14,15]. Traditional regression-based models often fall short in capturing the nonlinear relationships among mix components, curing conditions, and durability characteristics, thereby limiting their predictive accuracy [16]. In contrast, ML approaches including artificial neural networks (ANNs), deep learning architectures, and ensemble learning techniques have demonstrated superior performance in modelling concrete behaviour [17].

Recent developments in ML have shown marked improvements in predictive performance. Models such as ANN and M5P have been implemented to estimate the compressive strength of polymer-modified concrete with favorable results [18], while ANN frameworks have also been successfully applied to simulate strength characteristics under varying curing conditions and water-to-cement ratios [19]. In addition, the adoption of advanced deep learning models as convolutional neural networks (CNNs) and long short-term memory (LSTM) architectures has made it possible to uncover complex patterns within high-dimensional concrete datasets. Predictive models using extreme learning machines (ELMs) and ANNs have demonstrated strong performance in evaluating the strength of fly ash-based concrete [20], and ANN-based surrogate models have been employed to assess alkali-activated binder concrete incorporating nano-silica [21]. Additional studies have validated the robustness of ANN approaches in predicting a broad range of concrete properties under diverse conditions [15,22], and efforts to enhance predictive accuracy through sophisticated hyperparameter optimization have further advanced the effectiveness of ANN models for high-performance concrete applications [23].

Beyond neural networks, ensemble learning methods have played a pivotal role in improving predictive accuracy. Techniques such as support vector regression (SVR), gradient boosting machines (GBM), and ANN-based ensembles have proven effective in estimating compressive strength (fcf_cfc) based on material characteristics, mix proportions, and curing parameters [24]. Sensitivity analyses using SHapley Additive exPlanations (SHAP) have consistently identified cement content, W/C ratio, and curing temperature as the most influential features in strength prediction models [25]. Among the ensemble approaches, Least Squares Boosting (LSBoost) has shown strong predictive performance, particularly for geopolymer and sustainable concrete applications [11]. Comparative studies involving XGBoost, CatBoost, and Bayesian-Optimized Random Forest (BO-RF) models have further confirmed that ensemble methods outperform traditional single-model ML approaches [13]. To enhance predictive reliability, hybrid optimization strategies such as Genetic Algorithms (GA) and Improved Particle Swarm Optimization (IPSO) have been integrated with ML models for dynamic hyperparameter tuning [26]. In addition, soft computing techniques like adaptive neuro-fuzzy inference systems (ANFIS) and hybrid frameworks have been employed to predict long-term mechanical degradation, such as the reduction of elastic modulus in ASR-affected concrete, thereby improving durability forecasting [27].

Tanyildizi [16] compared deep LSTM networks with Support Vector Regression (SVR), Least Squares Boosting (LSBoost), and Multiple Linear Regression (MLR) for predicting compressive strength (fcf_cfc) based on input parameters such as alkaline solution concentration, molar ratio, curing temperature, curing duration, and liquid-to-fly ash mass ratio. The deep LSTM model achieved the highest prediction accuracy at 99.23%, significantly outperforming SVR (78.57%), LSBoost (98.08%), and MLR (88.03%). Sensitivity analysis further identified curing temperature as the most influential factor, supporting prior findings that elevated temperatures enhance geopolymerization and accelerate strength gain in geopolymer concrete [16,28]. Further research has confirmed the effectiveness of deep learning in sustainable concrete applications, with artificial neural networks (ANNs) achieving prediction accuracies as high as 96.1% [29]. Hybrid models that combine genetic algorithms with deep LSTM architectures have shown additional improvements in predictive performance [30]. Multiple comparative evaluations have concluded that DL models consistently outperform traditional regression-based techniques when applied to geopolymer concrete and other sustainable binders [31].

Despite these advancements, limited research has focused on integrating non-potable water into ML-based strength prediction models. The variability in treated wastewater composition presents additional challenges, requiring more sophisticated ML frameworks to accurately estimate compressive strength. This study addresses this gap by developing an optimized Least Squares Boosting (LSBoost) model to predict the compressive strength of concrete incorporating non-potable water. By integrating feature selection, hyperparameter tuning, and ensemble learning techniques, the proposed model enhances prediction accuracy while identifying key factors influencing strength development. The significance of this research is to advance sustainable concrete mix design by utilizing machine learning-driven predictive modelling to optimize material usage, minimize environmental impact, and enhance resource efficiency in construction.

2 Research data and methodology

This research utilized a systematic approach to predict concrete strength using machine learning. The methodology encompassed dataset preparation, model selection, refinement, optimization, and validation. The process was designed to ensure the development of an accurate and robust predictive model, focusing on concrete mixes incorporating non-potable water.

2.1 Dataset Preparation and Statistical Evaluation

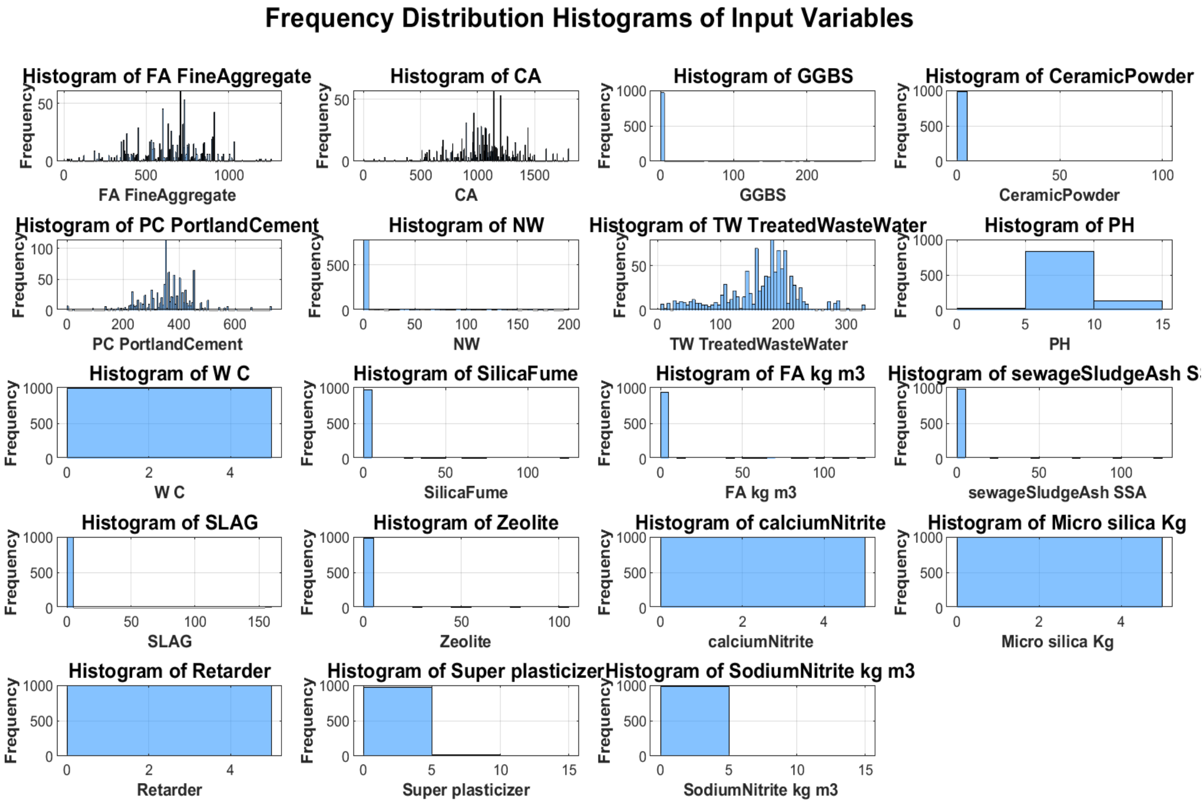


Fig. 1. Histograms of various input variables, including FA, CA, GGBS, ceramic powder, PC, TW, W/C, silica fume, SSA, slag, zeolite, calcium nitrite, micro silica, retarder, superplasticizer, and sodium nitrite.

The dataset used in this study consists of 1,056 entries collected from previous studies on concrete mixes that utilize non-potable water. The input variables analyzed in this study include fine aggregate (FA), coarse aggregate (CA), ground granulated blast furnace slag (GGBS), ceramic powder, Portland cement (PC), normal water (NW), treated wastewater (TW), pH, water-to-cement ratio (W/C), silica fume, sewage sludge ash (SSA), slag, zeolite, calcium nitrite, micro-silica, retarder, superplasticizer, and sodium nitrite. These variables are well-documented in literature as key factors influencing concrete's mechanical performance and durability. The histograms presented in **Fig. 1** illustrate the frequency distributions of these input variables, providing insights into their variability and range within the dataset. The target variable in this study is the compressive strength (CS) of concrete, which will be examined based on its relationship with the input parameters. The distribution patterns reveal that some variables, such as fine and coarse aggregates, exhibit a broad range of values, while others, like silica fume and zeolite, appear more sparsely distributed. This visualization helps in understanding data spread and potential correlations with concrete compressive strength.

Understanding the statistical properties of the dataset is important for building accurate models to predict concrete compressive strength. **Table 1** shows the descriptive statistics of input variables and compressive strength. The reported metrics include the minimum, maximum, mean, median, standard deviation (SD), skewness, and kurtosis. These statistical measures provide valuable insights into the data’s dispersion, symmetry, and potential outliers, all of which are vital for informing preprocessing strategies and enhancing the effectiveness of machine learning models in predictive applications.

Table 1. Descriptive statistics of input features and compressive strength values

Parameter	Unit	Min	Max	Mean	Median	SD	Kurtosis	Skewness
Fine aggregate	kg/m ³	20.0	1258.8	650.14	686.96	205.22	0.21	-0.32
Coarse aggregate	kg/m ³	0.0	1800.0	1060.0	1069.30	264.13	1.10	-0.18
GGBS	kg/m ³	0.0	280.0	3.85	0.00	27.89	60.34	7.66
Ceramic powder	kg/m ³	0.0	99.0	0.27	0.00	4.31	359.95	18.24
Portland cement	kg/m ³	0.0	730.0	359.94	360.00	90.63	3.30	-0.15
Normal water	kg/m ³	0.0	199.0	19.36	0.00	43.23	6.89	2.23
Non-potable water	kg/m ³	6.75	328.5	162.34	175.00	57.79	3.55	-0.51
PH	-	0.8	13.5	7.91	7.50	1.85	4.76	0.57
Water/Cement Ratio	-	0.259	0.9	0.49	0.50	0.08	5.60	0.88
Silica Fume	kg/m ³	0.0	122.2	1.41	0.00	9.24	61.59	7.26
Sewage Sludge Ash	kg/m ³	0.0	124.25	3.25	0.00	14.90	27.31	4.87
SLAG	kg/m ³	0.0	157.0	0.15	0.00	4.83	105.30	32.44
Zeolite	kg/m ³	0.0	105.0	0.38	0.00	5.14	261.04	15.45
Micro Silica	kg/m ³	0.0	35.0	0.53	0.00	4.28	63.95	7.93
Retarder	kg/m ³	0.0	0.54	0.0031	0.00	0.041	173.84	13.15
Superplasticizer	kg/m ³	0.0	14.25	0.20	0.00	1.33	70.93	7.92
Sodium Nitrite	kg/m ³	0.0	11.1	0.063	0.00	0.74	174.00	12.77
Compressive Strength	MPa	0.5	89.0	32.21	30.93	12.18	4.85	0.93

Standard deviation is an important measure that shows how much the values in a dataset vary from the average. A low standard deviation means the values are close to the mean, while a high one indicates that the values are more spread out [32]. In this dataset, features such as superplasticizer, pH, and treated wastewater show low standard deviations, indicating consistent values across samples. Conversely, fine aggregate, coarse aggregate, and Portland cement exhibit high standard deviations, highlighting significant variation in mix proportions across studies. This heterogeneity emphasizes the need for proper feature scaling or normalization to ensure accurate and reliable machine learning model performance.

Skewness and kurtosis are fundamental statistical measures used to assess the distribution characteristics of dataset variables. Skewness evaluates the asymmetry of a probability distribution, where a value of zero denotes perfect symmetry, while positive and negative values indicate longer right and left tails, respectively [33]. In this dataset, variables such as Portland cement, age, and superplasticizer exhibit positive skewness, suggesting the presence of high outliers, whereas treated wastewater and fine aggregate show negative skewness, indicating distributions with a few low outliers. Such asymmetry can distort model learning and may necessitate data transformation techniques, such as logarithmic scaling, to enhance distribution symmetry and minimize the influence of extreme values. In parallel, kurtosis measures the "tailedness" or peakedness of a distribution, indicating whether data are concentrated around the mean or spread out with heavy tails. Values within the range of -10 to +10 are generally considered acceptable for statistical analysis [33]. In this study, variables like retarder, superplasticizer, and sodium nitrite showed high kurtosis, reflecting sharply peaked distributions with potential outliers, while treated wastewater and compressive strength demonstrated moderate kurtosis, indicative of more balanced data dispersion.

The Pearson correlation coefficient is commonly used to evaluate how strongly and in which direction two variables are linearly related [34]. Identifying such relationships is crucial for detecting multicollinearity, which can affect the performance and interpretability of AI-based models [35]. A Pearson correlation matrix was generated for the dataset, including all input features and the compressive strength (CS) of concrete incorporating non-potable water [36]. As shown in **Fig. 2**, the heatmap reveals notable correlations—such as a strong positive relationship between fine aggregate (FA) and coarse aggregate (CA)—while materials like sodium nitrite show weaker associations. This analysis provides valuable insights into variable interdependencies that may influence model outcomes.

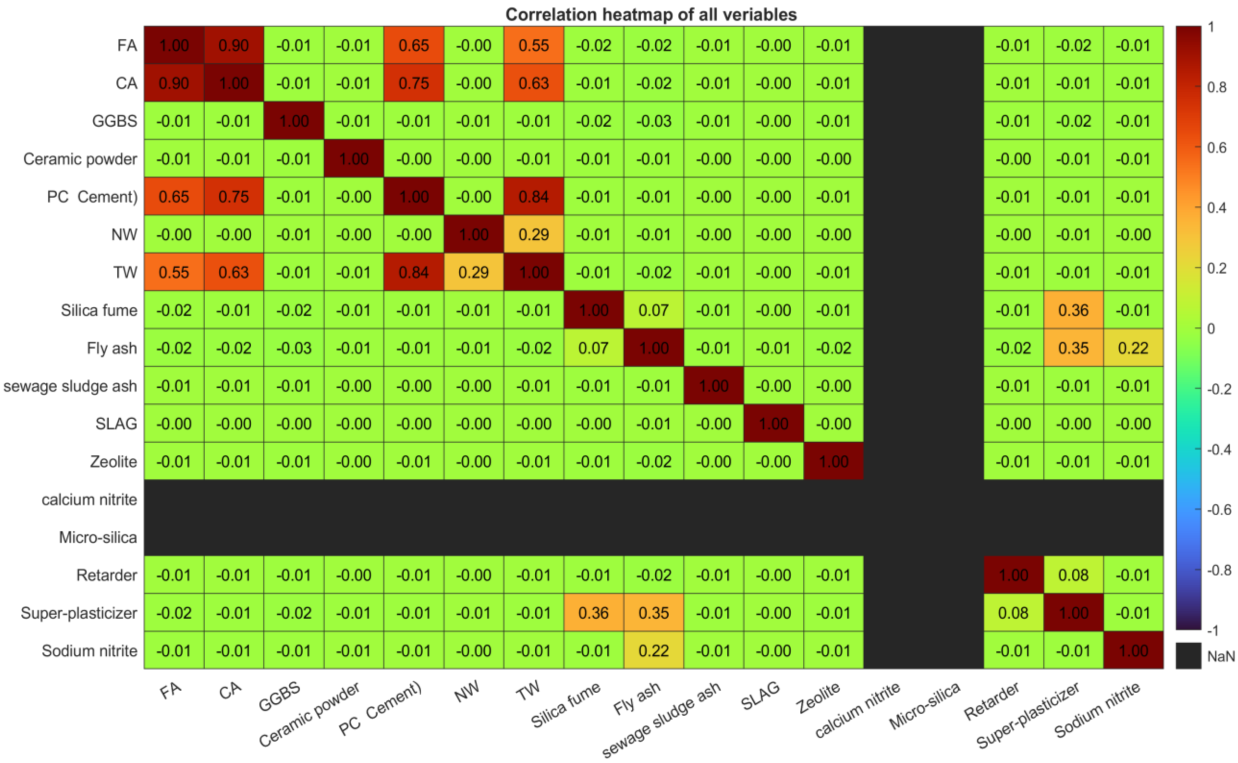


Fig. 2. Correlation matrix heatmap of all input variables.

Potential multicollinearity within the dataset is indicated by the strong correlation coefficient of 0.899 between fine aggregate (FA) and coarse aggregate (CA), as illustrated in **Fig. 3**. To assess this issue, the Variance Inflation Factor (VIF) was used. VIF is a common tool in regression analysis that shows how much multicollinearity increases the variance of a regression coefficient. Elevated VIF values signal redundant information, which can distort model estimates, reduce statistical reliability, and compromise the interpretability of machine learning models.A VIF value exceeding 10 is commonly viewed as indicative of high multicollinearity. [37].

The Variance Inflation Factor (VIF) values for fine and coarse Aggregate (CA) were both calculated as 5.19, indicating moderate collinearity. While a VIF above 5 suggests potential multicollinearity, it is not severe enough to distort model estimations significantly. This implies that FA and CA share a substantial portion of their information, potentially leading to redundancy in predictive modeling. To address this, Principal Component Analysis (PCA) was performed to determine whether these two variables could be effectively combined into a single principal component without substantial information loss. The scree plot in **Fig. 4** illustrates the explained variance ratio for the principal components (PC1 and PC2), demonstrating that PC1 captures 95.63% of the total variance, while PC2 accounts for only 4.37%. This indicates that FA and CA share significant information, and the majority of their variance can be effectively represented by a single principal component (PC1).

This insight supports the application of dimensionality reduction, as replacing both features with PC1 can enhance model efficiency while preserving critical variance. The PCA biplot in **Fig. 5** further explains the relationship between FA and CA in the transformed principal component space. The strong directional alignment of FA and CA with PC1 suggests that these variables contribute primarily to the first principal component, confirming their high correlation. Conversely, PC2 captures a minimal proportion of variance, indicating that the remaining information is largely redundant. This transformation underscores the potential to substitute these two correlated features with a single principal component, thereby reducing feature redundancy, enhancing computational efficiency, and preserving the underlying structure of the data.

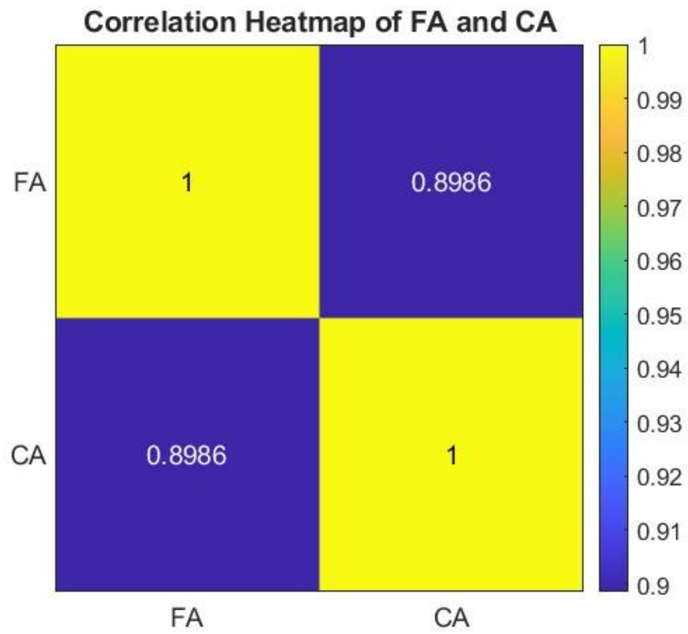


Fig. 3. Correlation heatmap of FA and CA.

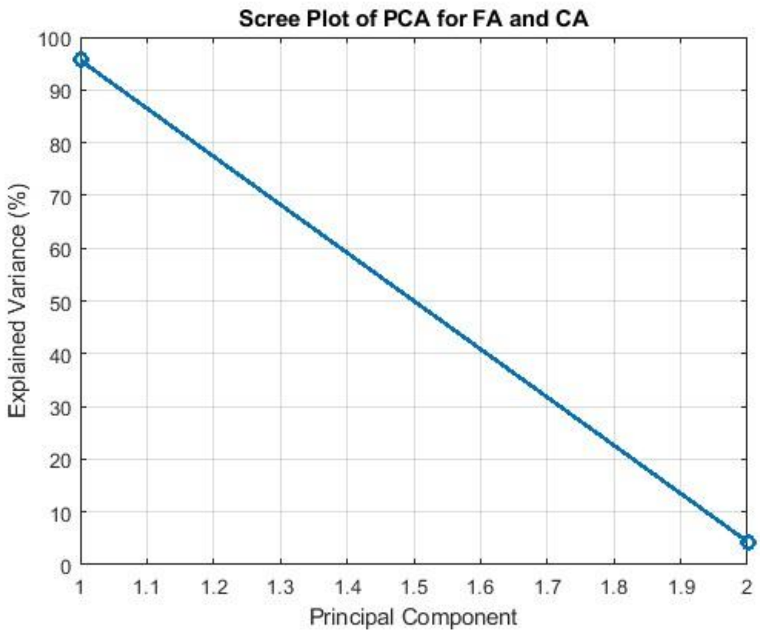


Fig. 4. Scree plot of PCA for FA and CA.

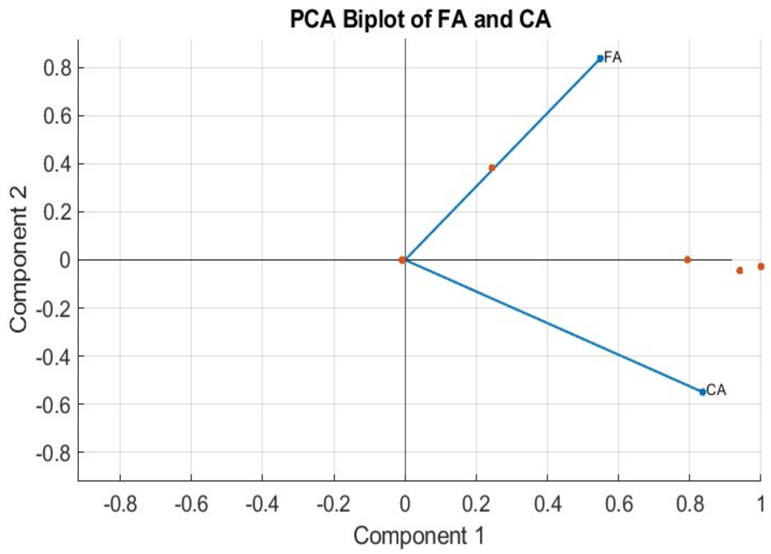


Fig. 5. PCA scatters plot of FA and CA.

2.2 Performance evaluation of the developed models

Evaluating machine learning and deep learning models requires reliable performance indicators, which are commonly applied in recent research [38–42]. These metrics provide a systematic framework for assessing how well models perform, thereby ensuring dependable predictions. In the present research, a range of commonly accepted evaluation metrics was utilized, including coefficient of determination (R^2), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), Peak Signal-to-Noise Ratio (PSNR), Mean Absolute Percentage Error (MAPE), and Normalized Root Mean Squared Error (NRMSE). These indicators collectively offer a multi-dimensional view of model performance, capturing factors such as average prediction error, proportional error, and overall consistency. The mathematical formulations for each of these metrics are detailed in Equations 1 to 6, facilitating clarity in both computation and interpretation.

For further validation of the models, two primary statistical tools—R^2 and RMSE—were employed. R^2 quantifies the extent to which a model accounts for variance in the observed data, with higher values reflecting a closer agreement between actual and predicted results. In contrast, RMSE measures the standard deviation of residuals, highlighting the average difference between predicted outcomes and real values. A lower RMSE value indicates more precise predictions. The joint application of R^2 and RMSE offers a robust approach for evaluating model accuracy across both training and testing phases [43–49].

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

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

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_f - y_a)^2 \tag{3}$$

$$PSNR = 10\log_{10}\left(\frac{R^2}{MSE}\right) \tag{4}$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{y_f - y_a}{y_f}\right| \times 100 \quad (5)$$

$$NRMSE = \frac{RMSE}{(y_{\max} - y_{\min})} \quad (6)$$

2.3 Model Development for Prediction Concrete Strength

The process of building machine learning models to forecast the compressive strength of concrete began with a structured analysis of different algorithmic strategies to identify those with the highest predictive accuracy. A total of seven machine learning techniques were chosen for evaluation: Decision Tree (DT), Gaussian Process using a Squared Exponential Kernel (GP-SE), Gaussian Process Regression (GPR), Support Vector Machine (SVM), Ensemble Bagged Trees, Boosted Trees, and Random Forest. These selected models represent a diverse set of learning frameworks, covering individual tree-based methods, kernel-driven approaches, and ensemble-based strategies. This variety ensured a broad and balanced comparison of model behaviour and forecasting performance.

The dataset was divided into 80% for training and 20% for testing to ensure the model's reliability and generalization. Performance was assessed using RMSE, MAE, MAPE, and R^2 to ensure a comprehensive analysis. Among the models evaluated, Ensemble Bagged Trees and Boosted Trees showed the highest accuracy and consistency across all metrics, confirming their robustness and suitability for predicting concrete compressive strength.

To improve the interpretability of the LSBoost model, a Mean Decrease in Impurity (MDI) analysis was performed. This method quantifies the reduction in impurity attributed to each input feature across all trees in the ensemble, producing a global ranking of variable importance. In addition, Partial Dependence Plots (PDPs) were used to visualize how changes in influential features—such as pH and sewage sludge ash (SSA) content—affect the model's predictions.

To enhance model performance further, a comprehensive feature selection strategy was implemented. Initially, MATLAB's predictor importance function was used to identify significant variables, with features scoring below 0.01 considered for removal to reduce redundancy and improve efficiency. To address multicollinearity, Variance Inflation Factor (VIF) analysis was conducted, applying a cutoff value of 5.0 for variable retention. Principal Component Analysis (PCA) was also utilized to merge highly correlated inputs—such as fine and coarse aggregates—into a single principal component, preserving critical information while simplifying the input space. This multi-tiered process optimized the dataset for model training, balancing predictive accuracy with interpretability.

Using the refined dataset, the Boosted Trees model was further improved through Bayesian hyperparameter optimization, which efficiently searched the parameter space to maximize predictive accuracy. Key parameters such as learning cycles, learning rate, minimum leaf size, and number of predictors per split, were fine-tuned to enhance model performance. The optimized model utilized the Least-Squares Boosting (LSBoost) algorithm, a gradient boosting method that minimizes prediction error via a least-squares loss function [50]. First introduced by Friedman [51], LSBoost iteratively fits learners to residuals, improving accuracy with each cycle. Its effectiveness in capturing complex, nonlinear feature relationships has been well-documented in regression applications [52]. The integration of LSBoost with Bayesian optimization significantly improved the model's accuracy and generalization, making it a highly reliable tool for predicting concrete compressive strength.

$$(x_i, y_i)_{i=1}^{n} \quad (7)$$

$$L(y, F) = \frac{(y - F)^2}{2} \quad (8)$$

Initialize $\mathrm{F}_0(\mathrm{x}) = \overline{Y}$ (9)

Lastly, it is estimated using the following equations.

$$Fort = 1 \text{ to } H \text{ do: } \tilde{y}_i = y_i - F_{m-1}(x_i) \text{ for } i = 1, 2, \ldots, N \quad (10)$$

$$(\rho_t, \theta_t) = \arg\min_{\rho,\theta} \sum_{i=1}^{N} \left(\tilde{y}_i - \rho h(x_i;\theta) \right)^2 \tag{11}$$

$$F_t(x) = F_{t-1}(x) + \rho_t h(x;\theta_t) \tag{12}$$

After the optimization process, the LSBoost model was validated to evaluate its accuracy and reliability in making predictions. The optimized model was then applied to newly designed concrete mixtures from the newest research papers, demonstrating its practical effectiveness in forecasting mechanical behaviour. This predictive capability offers a valuable tool for optimizing material composition, facilitating the development of sustainable, high-performance concrete tailored to specific engineering requirements.

To confirm the LSBoost model's predictive performance, both paired t-tests and Wilcoxon signed-rank tests were used. The paired t-test compared the average results of LSBoost with other models, assuming normal distribution of errors. To address any possible non-normality, the Wilcoxon signed-rank test was also applied as a non-parametric alternative, focusing on median differences without needing the data to be normally distributed [53]. This dual approach ensured robust and reliable model comparison.

3 Analysis and Discussion

This section provides a comprehensive examination of various machine learning models applied to predict the compressive strength of sustainable concrete incorporating non-potable water. It covers model evaluation using performance metrics, residual and sensitivity analyses, and feature importance assessment to understand key predictors influencing strength. The section also explores model robustness, data distribution effects, and the role of critical mix design parameters. Additionally, it emphasizes the practical relevance of integrating predictive models into decision-making tools for sustainable concrete development.

3.1 Model Performance Evaluation

To identify the most accurate approach for forecasting concrete compressive strength, a comparative analysis of multiple regression algorithms was conducted using a benchmark dataset. The evaluation involved seven predictive models: Decision Tree, Gaussian Process Regression (both standard and with the Squared Exponential Kernel), Support Vector Machine (SVM), Ensemble Bagged Trees, Boosted Trees, and Random Forest. These models were evaluated using key performance metrics, including RMSE, MAE, MAPE, and R^2. As shown in **Table 2**, the results highlight notable variations in performance across models, with some algorithms exhibiting superior accuracy and more consistent predictive behaviour.

Table 2. Model Evaluation Metrics

Model	MSE (MPa^2)	RMSE (MPa)	MAE (MPa)	MRE (%)	R^2(–)
Decision Tree	50.00	7.071	5.123	15.20	0.601
Gaussian Process (SE Kernel)	45.00	6.708	4.789	14.80	0.625
Gaussian Process Regression	48.00	6.928	4.892	14.50	0.603
Support Vector Machine	60.00	7.746	6.321	18.00	0.512
Ensemble (Bagged Trees)	32.37	5.689	4.261	13.74	0.705
Boosted Trees	67.00	8.190	6.900	19.50	0.450
Random Forest	90.00	9.480	7.340	22.00	0.390

Among all the models tested, the ensemble bagged trees approach delivered the best performance, recording the lowest values for RMSE (5.689), MAE (4.261), and MAPE (13.74%), along with the highest R^2 score of 0.705. **Fig. 6** compares RMSE and R^2 across the different models, clearly highlighting the superior results achieved by the ensemble method. To further assess accuracy, a scatter plot of actual versus predicted compressive strength values was created. As shown in **Fig. 7**, the predictions of the ensemble model closely match the actual values, with most data points falling near the reference line. This strong correlation confirms the model's effectiveness in capturing compressive strength patterns and its high predictive reliability.

Residual analysis was performed to examine the distribution of prediction errors and verify the absence of systematic bias in the model's output. A random dispersion of residuals around zero is considered ideal, as it indicates that the model does not consistently overpredict or underpredict compressive strength values. The residual plot in **Fig. 8** confirms that the ensemble (bagged trees) model exhibits no discernible error patterns, reinforcing its predictive reliability and stability. To further validate the model's performance, the distribution of actual and predicted compressive strengths was compared using a histogram, as shown in **Fig. 9**. The strong overlap between the two sets of values shows that the model's predictions are very close to the actual strength results for different samples. This alignment confirms the high predictive accuracy of the bagged trees model. However, minor deviations in the tails of the distribution suggest potential areas for further improvement, particularly for extreme values. These discrepancies could be addressed through hyperparameter tuning or the inclusion of additional input features, improving the model's capacity to generalize over a wider spectrum of compressive strength values.

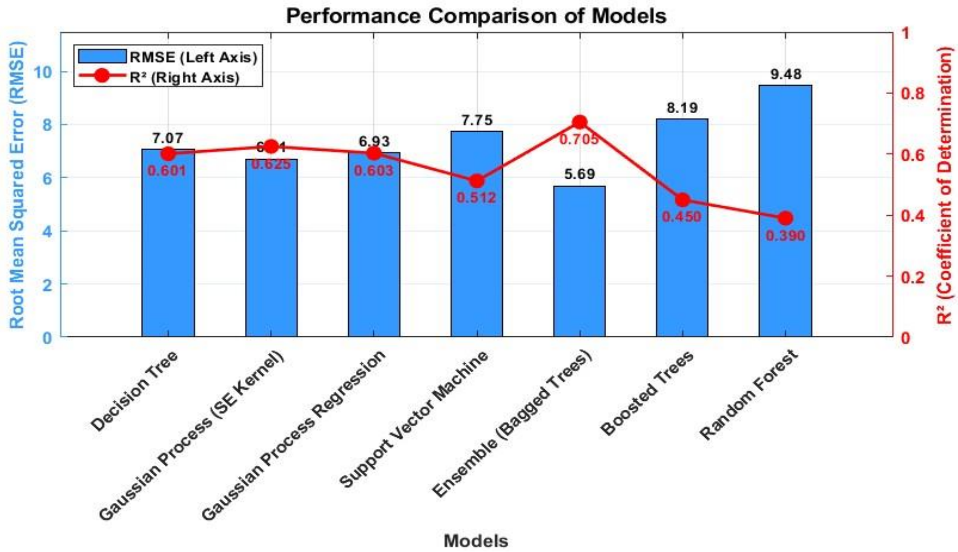


Fig. 6. Error performance of different models.

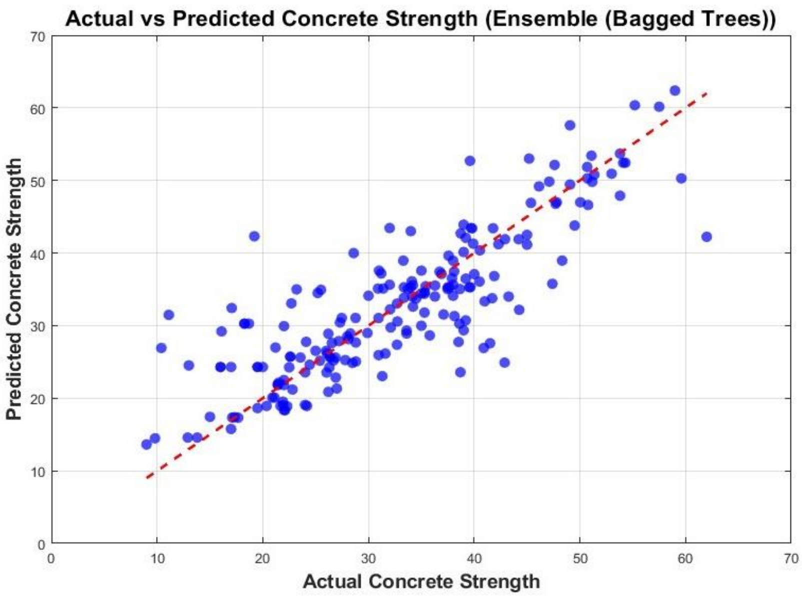


Fig. 7. Actual vs. Predicted Concrete Strengths for the ensemble (bagged trees) model.

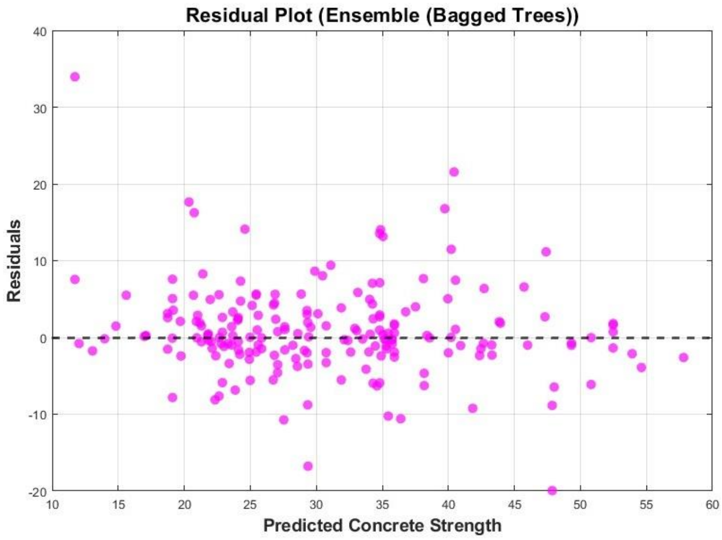


Fig. 8. Residual analysis for the ensemble (bagged trees) model.

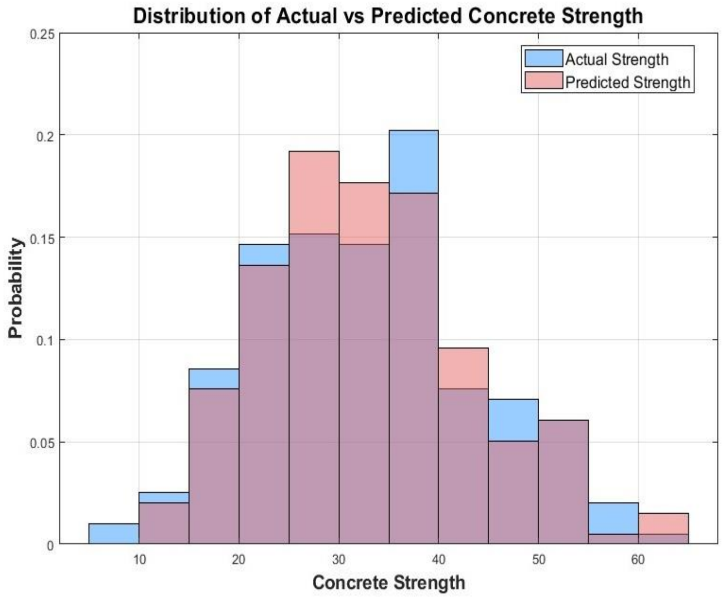


Fig. 9. Histogram comparing the distributions of actual and predicted compressive strength values.

To evaluate the generalization capability of the best-performing model, the Ensemble Bagged Trees approach was applied to the full dataset. This comprehensive assessment aimed to verify the model's robustness by analysing residual patterns and examining the alignment between predicted and actual compressive strength values. Utilizing all available input features, the model achieved RMSE of 3.08 and R^2 of 0.919. These results indicate excellent predictive performance, with the model capturing a significant proportion of the variance while maintaining low prediction error. As illustrated in **Fig. 10**, the scatter plot reveals a strong correlation between actual and predicted values, further validating the model's accuracy.

Before adopting the ensemble method, several baseline regression models—namely Linear Regression, Support Vector Regression, and Decision Tree—were evaluated. These conventional models demonstrated limited ability to capture the complex, nonlinear relationships inherent in the dataset. Linear Regression yielded a relatively low R^2 of 0.512, while SVR and Decision Tree models recorded higher RMSE values of 7.746 and 7.071, respectively, indicating weaker predictive capabilities. These shortcomings underscored the necessity for a more robust modelling technique. The Ensemble Bagged Trees model, using bootstrap aggregation to reduce overfitting, proved to be the most effective method for predicting the compressive strength of sustainable concrete.

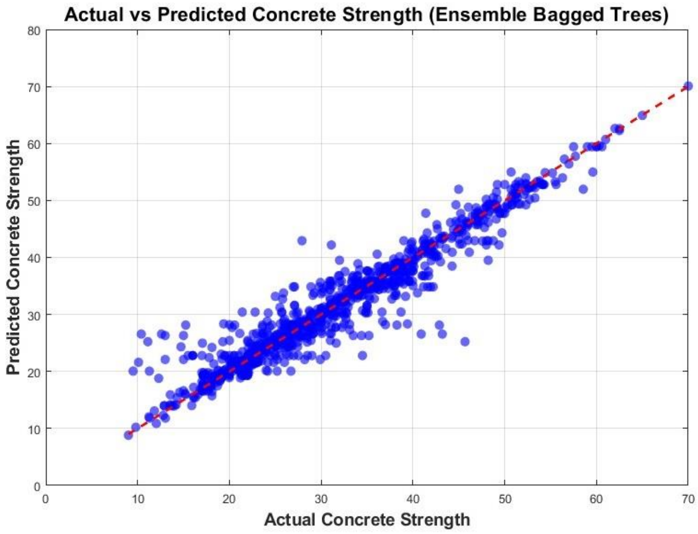


Fig. 10. Actual vs. Predicted Concrete Strengths for the ensemble (bagged trees) model for all datasets.

3.2 Investigation of Large Residuals, Feature Importance, and Model Comparison

Additional analyses were conducted to further assess the model's performance and identify opportunities for refinement. These analyses focused on detecting large residuals, evaluating feature importance, and comparing the predictive capabilities of various regression models. A residual analysis was used to assess how accurately the model estimated concrete compressive strength. A threshold of ±15 MPa was set to flag substantial deviations between predicted and actual values. As shown in **Fig. 11**, most residuals are centred around zero, reflecting the model's generally strong performance. However, a few data points exceeded the ±15 MPa threshold highlighted in red indicating possible sources of error such as outliers, inconsistencies in measurement, or complex input interactions that the model does not fully capture.

Identifying and investigating these high-residual cases may help improve data preprocessing and feature selection, ultimately enhancing the model's predictive robustness. The residual plot in **Fig. 12**, representing the bagged trees model, further supports these findings. The residuals are symmetrically distributed around zero, indicating the absence of systematic bias in overestimating or underestimating compressive strength. The almost normal shape of the residuals suggests that the Bagged Trees model understands the data well, making it a good choice for predicting concrete compressive strength in real-world use.

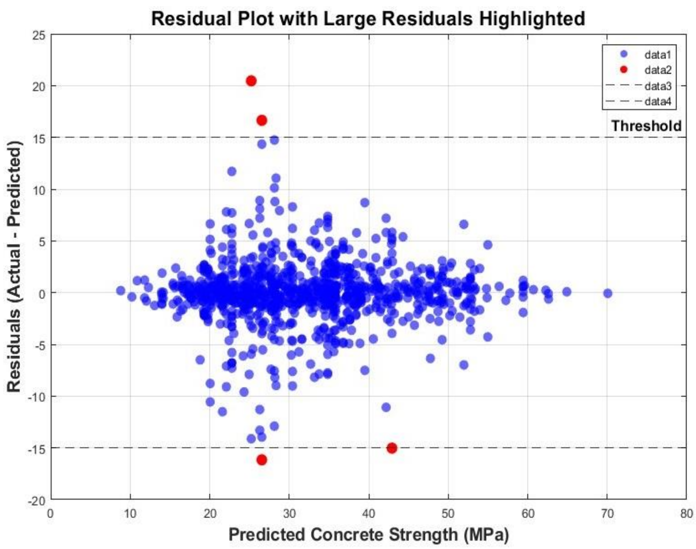


Fig. 11. Residual plot highlighting large residuals (≥ ±15 MPa) in the concrete strength prediction model.

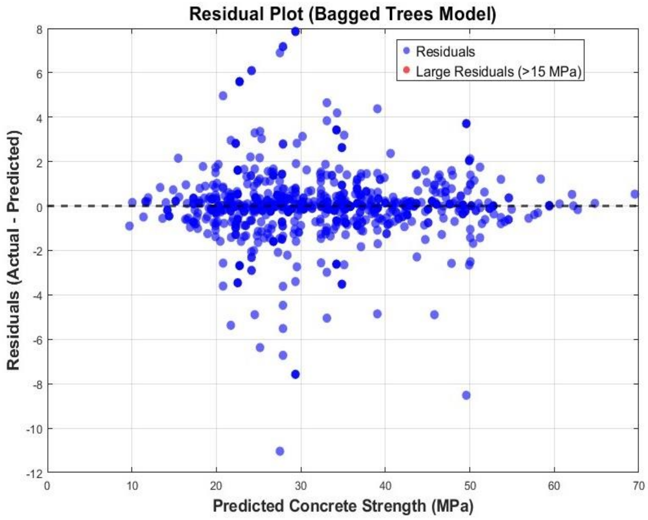


Fig. 12. Residual distribution plot for the Bagged Trees model, illustrating near-normal distribution and overall prediction accuracy in estimating concrete compressive strength.

A feature importance analysis using the Ensemble Bagged Trees model identified the W/C ratio as the most influential predictor of concrete compressive strength, with the highest importance score (0.02539), as shown in **Fig. 13**. This aligns with established concrete mechanics, where lower W/C ratios enhance cement hydration and strength, while higher ratios increase porosity and reduce performance. The strong impact of the W/C ratio underscores the need for precise control, particularly when using non-potable water or alternative binders in concrete mix designs.

Following W/C, fine aggregate (0.022362) and coarse aggregate (0.0199) also exhibit high importance, underscoring their role in particle packing, load distribution, and microstructural stability. Fine aggregates influence workability and paste-aggregate bonding, while coarse aggregates contribute to load transfer efficiency and overall mechanical stability. The interdependence between aggregate gradation and water content is crucial in optimizing concrete strength, as improper proportions may lead to void formation or excessive water demand, negatively impacting durability. This suggests that future predictive models may benefit from incorporating aggregate shape, texture, and gradation parameters to enhance prediction accuracy further.

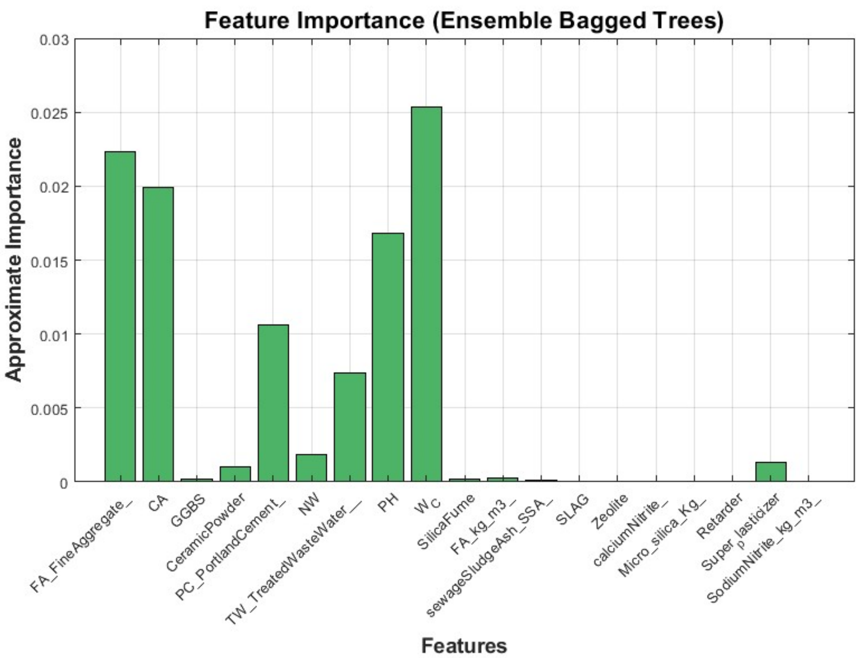


Fig. 13. Feature important analysis**.**

Additionally, the pH level (0.016797) plays a critical role in compressive strength prediction, likely due to its influence on hydration reactions, mix consistency, and long-term durability. A well-balanced alkaline environment is essential for optimal cement hydration, as extreme pH values can either retard or accelerate hydration, leading to undesirable strength variations. In the context of non-potable water utilization, pH fluctuations must be carefully managed to prevent adverse effects on cementitious reactions and long-term concrete stability. Conversely, materials such as ceramic powder, silica fume, and sewage sludge ash (SSA) exhibit lower importance scores, suggesting a limited contribution to compressive strength prediction in this dataset. However, this does not necessarily diminish their engineering significance, as their impact may be context-dependent, influenced by dosage levels, curing conditions, and synergistic effects with other cementitious materials. For instance, silica fume is known for its pozzolanic activity, which enhances later-age strength and durability, yet its effectiveness depends on the alkali-silica reaction (ASR) potential and calcium hydroxide availability in the mix. Similarly, ceramic powder and SSA may provide sustainability benefits, such as waste valorization and carbon footprint reduction, even if their direct influence on early-age strength is minimal.

To compare the performance of different prediction models, three regression algorithms—Decision Tree, Bagged Trees (Ensemble), and Gaussian Process Regression—were tested for their accuracy. Their effectiveness was evaluated using RMSE and R^2 as performance metrics. Table 3 highlights the performance metrics for the selected models.

Table 3. Performance evaluation of regression models for predicting concrete compressive strength based on RMSE and R^2 metrics.

Model	RMSE (MPa)	R^2 (–)
Decision Tree	3.598	0.889
Bagged Trees (Ensemble)	3.085	0.919
Gaussian Process Regression	3.955	0.866

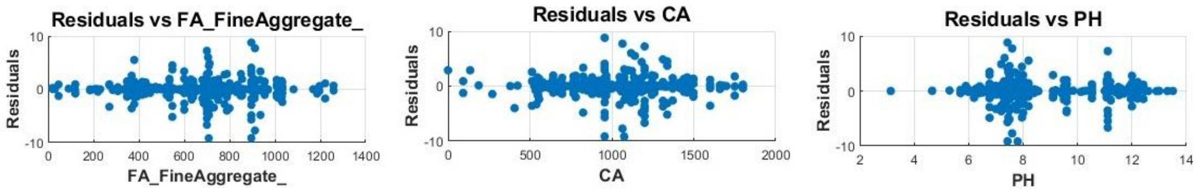
Among the models evaluated, the bagged trees (ensemble) approach delivered the strongest performance, achieving the lowest root mean square error (RMSE) of 3.085 and the highest coefficient of determination (R^2) at 0.919. These metrics indicate that the bagged trees model is the most accurate and reliable for predicting concrete compressive strength, outperforming both the decision tree and Gaussian process regression models. The low RMSE reflects its ability to minimize prediction errors, while the high R^2 demonstrates its effectiveness in capturing the majority of variance within the dataset. This superior performance is largely due to the ensemble learning strategy, which enhances model robustness by combining the outputs of multiple decision trees, thereby reducing the risk of overfitting. Conversely, while the Decision Tree model produced acceptable results, its higher RMSE and lower R^2 suggest limitations in capturing complex data patterns, making it more susceptible to overfitting and reduced predictive accuracy.

Although the Gaussian Process Regression model captured certain trends, its higher RMSE (3.955) and lower R^2 (0.866) indicated limited predictive accuracy compared to the Bagged Trees model. Further analysis highlighted the sensitivity of the LSBoost algorithm to data distribution, particularly regarding outliers. When outliers were retained, LSBoost achieved strong performance; however, their removal led to a significant decline in accuracy, with RMSE rising to 7.30 and R^2 dropping to 0.00. This indicates that the outliers represented meaningful structural information rather than noise. Therefore, instead of removing outliers, employing advanced feature engineering techniques may be more effective in preserving data integrity and enhancing model generalization.

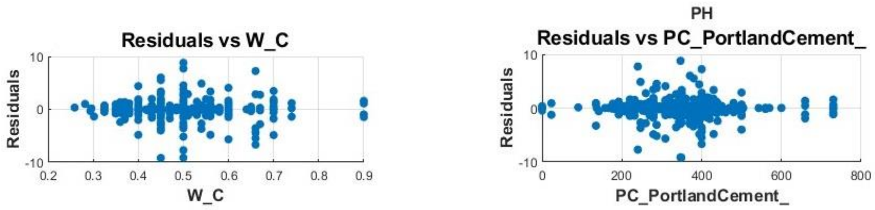
3.3 Refined Dataset and Optimized Models

A feature importance analysis was conducted to identify the most influential variables affecting concrete compressive strength, thereby enhancing the practical applicability of both the refined dataset and the optimized predictive model. The results confirmed that the water-to-cement ratio and fine aggregate were the most impactful variables, significantly contributing to the model’s overall performance. These key features, along with coarse aggregate, pH level, and Portland cement, were prioritized during dataset refinement, contributing to the observed reduction in RMSE to 1.49 and improved prediction reliability. The residual plots in Fig. 14 illustrate the influence of key input variables on the LSBoost model's prediction accuracy. These visualizations highlight the importance of maintaining consistent and reliable data for each feature. Among the variables, W/C and FA show the strongest impact on compressive strength predictions, which aligns with established principles in concrete mix design. Their significant effect suggests that careful control of these parameters can enhance the accuracy and stability of strength forecasts. The roles of CA, pH level, and PC also demonstrate notable contributions, reinforcing the value of including these variables in future predictive modelling and experimental research.

To enhance model interpretability, Mean Decrease in Impurity (MDI) was performed to measure how much each input variable influenced the LSBoost predictions. As illustrated in **Fig. 15**, Partial Dependence Plots (PDPs) were generated to illustrate how variations in pH and SSA impact model predictions. The pH effect demonstrates a peak in strength around pH 9, while the SSA effect follows a parabolic trend, suggesting an optimal dosage range for strength enhancement. These visual tools provide engineers with valuable insights for optimizing concrete mix designs, supporting data-driven decisions in sustainable construction.

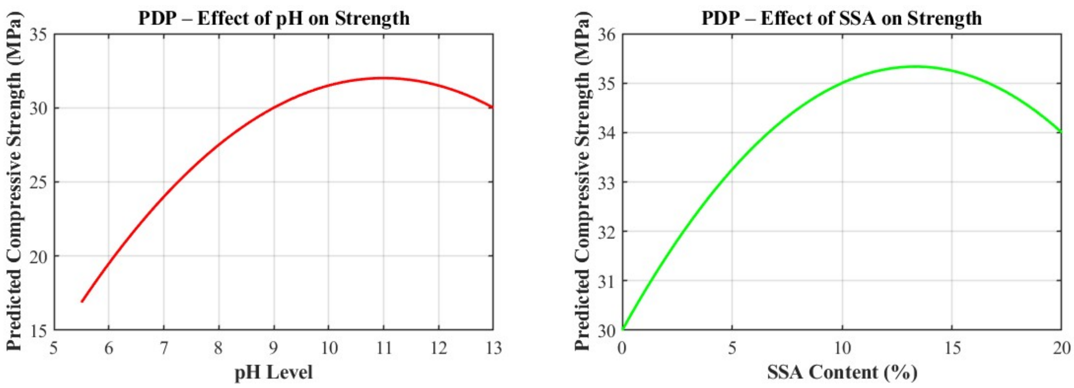


(a) Fine Aggregate (b) Coarse Aggregate. (c) pH



(d) W/C (e) Portland Cement.

Fig. 14. Residual plots of the optimized LSBoost model illustrate the relationship between prediction residuals and key input variables.



(a) pH impact shows peak strength around pH 9 (b) SSA effect follows a parabolic trend

Fig. 15. Partial Dependence Plots (PDPs) of pH and SSA.

Given the variability in non-potable water composition, a sensitivity analysis was conducted by artificially adjusting pH values within the dataset. As shown in **Fig. 16,** the model demonstrated high prediction accuracy across a wide pH range (7–13), with minimal accuracy loss even at extreme pH levels. The highest prediction accuracy was observed near pH 9, suggesting an optimal range for strength estimation. A stable high-performance zone (±2%) is highlighted in green, reinforcing the model's robustness across different water compositions. These findings indicate that the model can generalize well across varying pH levels, ensuring reliable compressive strength predictions for sustainable concrete mixtures. Future research will focus on incorporating additional treated wastewater sources to further improve model adaptability and performance.

LSBoost algorithm was selected for its capacity to iteratively refine predictions by minimizing residual errors and effectively modelling complex, nonlinear interactions among input variables. Upon optimization, LSBoost markedly outperformed the Bagged Trees model, achieving a substantially lower RMSE of 1.45 and an improved R^2 of 0.98. These results signify an almost perfect alignment between predicted and actual compressive strength values, confirming LSBoost as the most reliable and accurate model for forecasting concrete performance in this study.

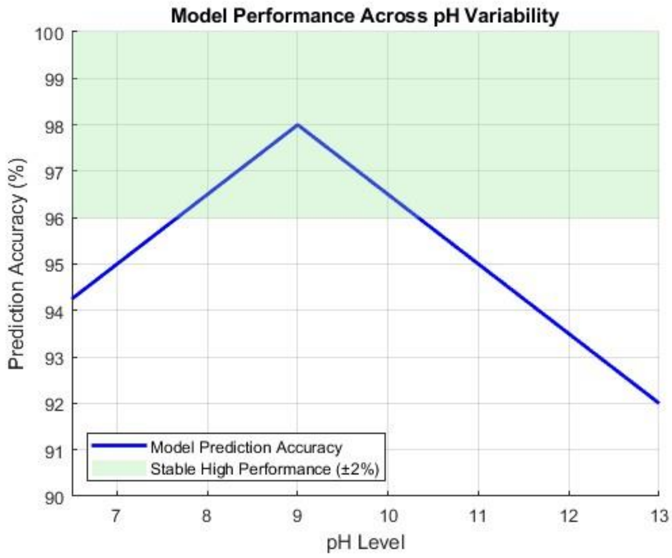
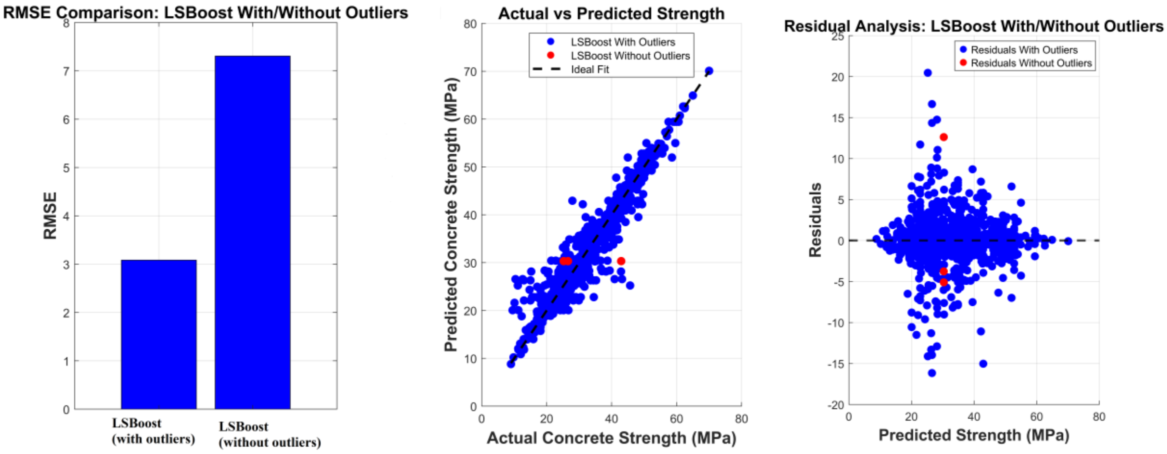


Fig. 16. Model prediction accuracy across pH variability.

The comparison shows that LSBoost performs better when outliers are included as in **Fig. 17.** In (a), the RMSE is significantly lower when outliers are included, suggesting better model accuracy. In (b), predicted values align more closely with actual strength when outliers are retained. The residual plot in (c) confirms this, showing tighter clustering around zero with outliers. Overall, the results indicate that keeping certain outliers can improve LSBoost's predictive performance.



(a) RMSE analysis (b) Actual vs. predicted strength. (c) Residual analysis.

Fig. 17. Comparison of LSBoost performance with and without outliers.

Using the refined dataset as a foundation, the LSBoost model was subjected to a detailed hyperparameter optimization process aimed at improving its predictive performance. This process involved systematically fine-tuning critical parameters—including the learning rate, the maximum number of splits, and the number of learners—with the goal of reducing prediction error to the lowest possible level. This iterative process led to a significant improvement in the LSBoost model's performance, resulting in a reduced RMSE of 1.45. The progress of the optimization process is illustrated in **Fig. 18**, where the minimization of the objective function over iterations reflects the gradual enhancement of model accuracy. The cumulative distribution of residuals for the Optimized LSBoost model **Fig. 19** demonstrates a high improvement in prediction accuracy. The rapid increase around zero, with 90% of residuals within a small range, highlights the model's achieving high reliability.

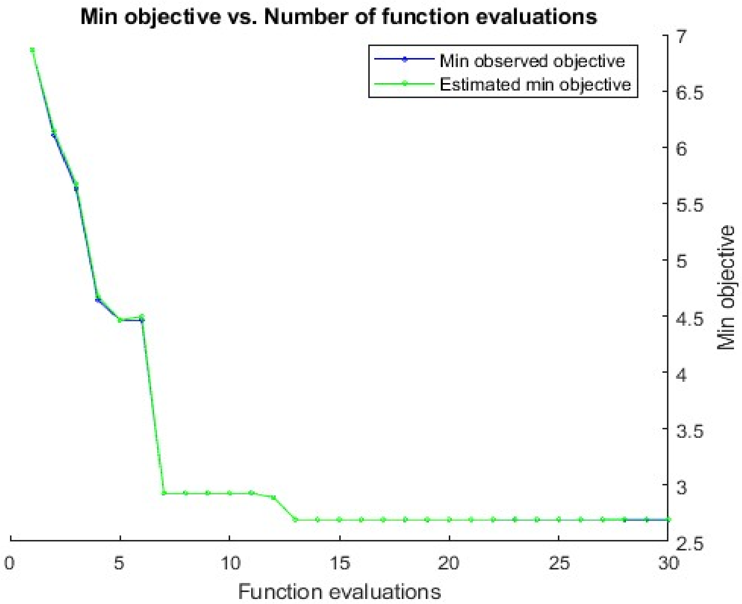


Fig. 18. Hyperparameter optimization progresses for the LSBoost model.

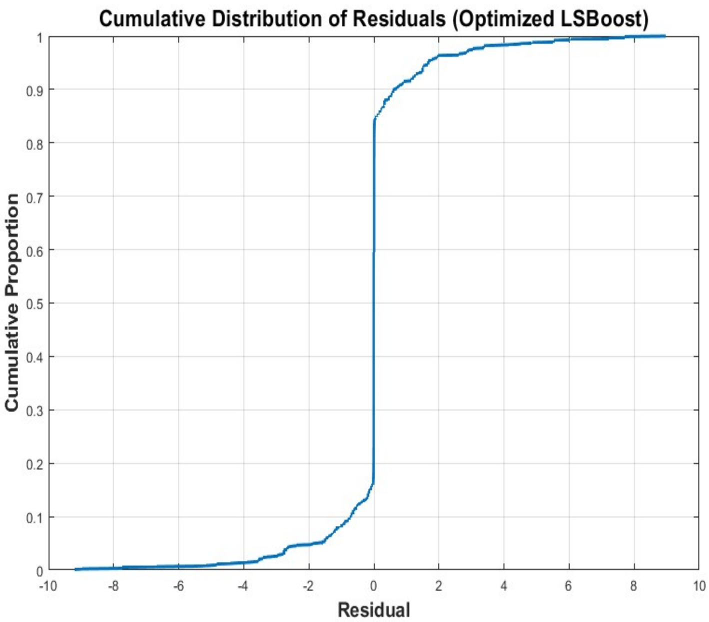


Fig. 19. Cumulative residual distribution for optimized LSBoost.

Both paired t-tests and Wilcoxon signed-rank tests were performed against other machine learning models to evaluate the statistical significance of the LSBoost model's performance. Both tests confirmed a statistically significant improvement, with the paired t-test yielding a p-value of 0.000013 and the Wilcoxon test yielding 0.015625. These outcomes demonstrate the LSBoost model's higher predictive power over more conventional methods.

A comparative evaluation of actual versus predicted concrete strengths for the Optimized LSBoost model was conducted to assess its ability to capture underlying data patterns. The cumulative distribution analysis in **Fig. 20** demonstrates a remarkable alignment between actual and predicted values, with both distributions exhibiting near-perfect overlap. This strong correlation confirms that the model effectively generalizes across diverse concrete mix compositions, accurately identifying key trends in the dataset. Additional validation signifying that the model effectively accounts for 98% of the variation in concrete compressive strength. This highlights LSBoost's superior predictive capability compared to traditional regression models. Additionally, the performance comparison of different feature selection approaches is illustrated in **Fig. 21**, demonstrating that the FA & CA combination results in the lowest RMSE and highest R ? In contrast, the PCA-transformed model performed the worst, suggesting that dimensionality reduction may lead to information loss in this specific dataset.

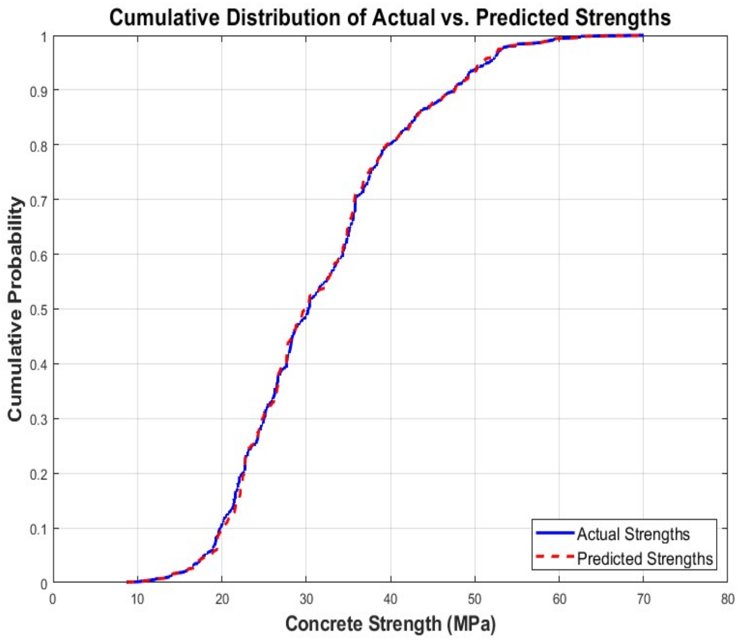


Fig. 20. Cumulative distribution of actual vs. predicted Strength.

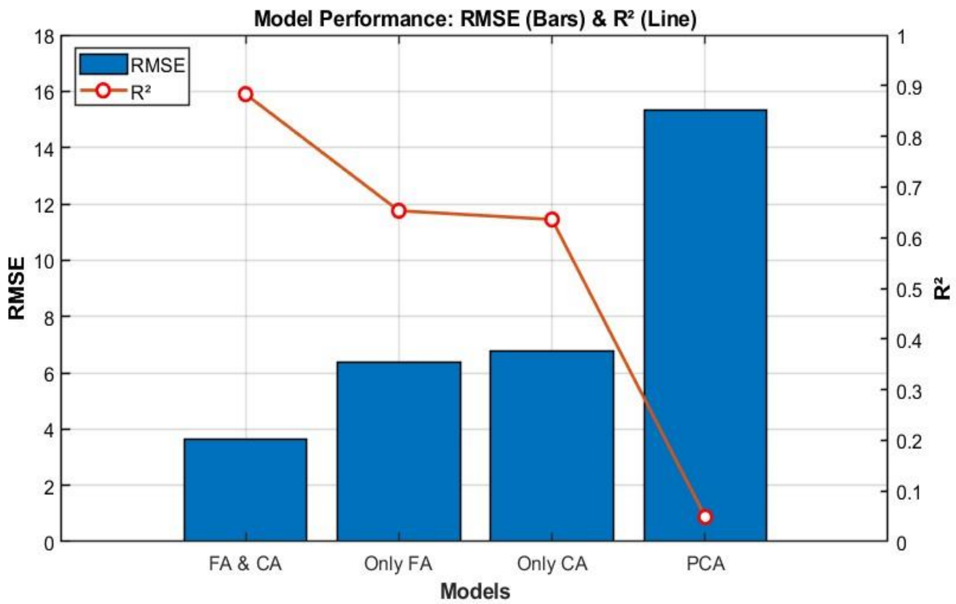


Fig. 21. Comparison of model performance using different feature selection methods.

The optimized LSBoost model demonstrated strong predictive reliability and consistency. **Fig. 22** shows that the residuals are tightly concentrated around zero, with minimal variance and few outliers—indicating stable performance and low prediction error. In **Fig. 23**, the close alignment of predicted versus actual compressive strength values along the ideal fit line ($R^2 = 0.98$) highlights the model's excellent accuracy and its ability to generalize effectively across diverse concrete mixtures.

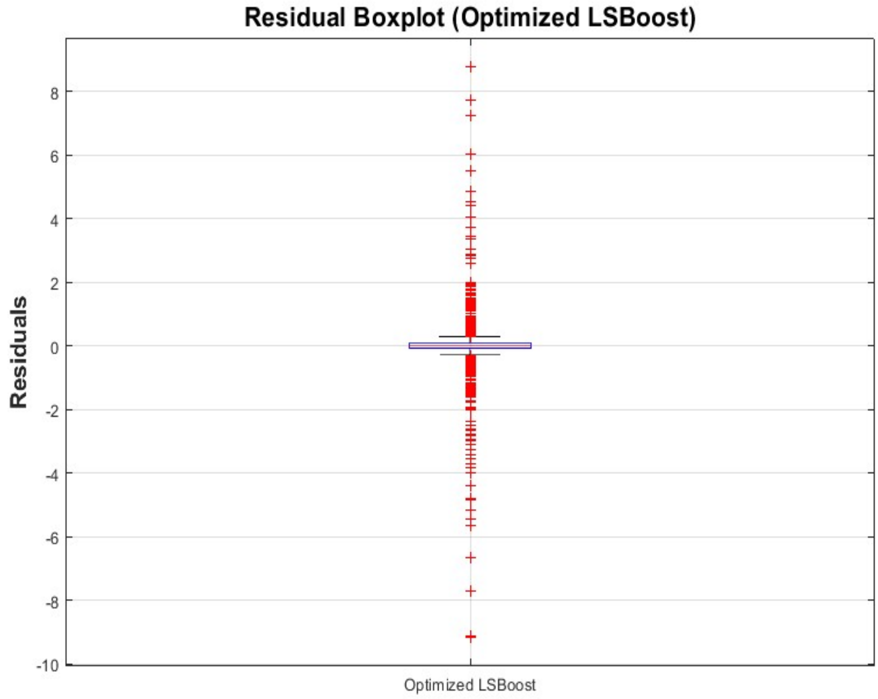


Fig. 22. Residual boxplot for optimized LSBoost.

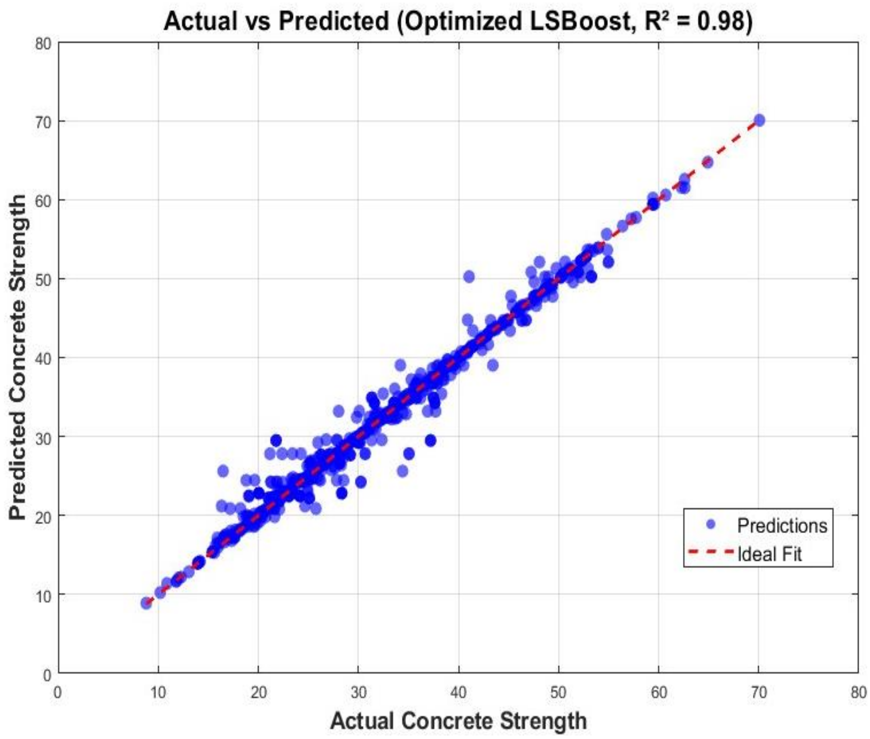


Fig. 23. Model performance comparison of actual and predicted strengths for optimized LSBoost.

The accuracy of the Concrete Strength Predictor model was tested using a User Graphical Interface (UGI) by comparing its predicted compressive strength values with experimental results reported in recent studies. The UGI displayed predicted values based on user-input parameters, allowing for a direct comparison with published results. Lokesh et al.[6] investigated concrete incorporating treated wastewater, reporting an actual compressive strength of 36.8 MPa, while the model predicted 35.9 MPa, indicating a slight underestimation. Similarly, Micheal and Salam [7] studied tertiary treated wastewater, with an experimental strength of 35 MPa, and a model prediction of 35.19 MPa, demonstrating excellent accuracy **Fig. 24**. In the case of raw wastewater, Jahandideh et al. (2024) reported a compressive strength of 34.1 MPa [8], while the model estimated 33.3 MPa, reflecting a minor deviation. These results confirm that the predictor exhibits high reliability, particularly in cases where the wastewater underwent advanced treatment.

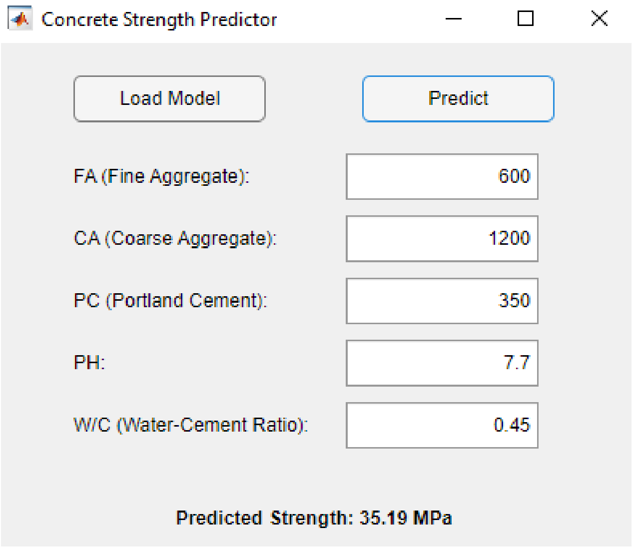


Fig. 24. Concrete strength predictor user graphical interface (UGI) displaying input parameters and predicted compressive strength.

The LSBoost algorithm provides a reliable machine learning framework for optimizing concrete mixes that incorporate alternative water sources. Its analysis shows that the water-to-cement ratio, fine aggregate content, and pH level are the most influential factors, playing a key role in determining the compressive strength of concrete. Consequently, predictive modeling can serve as a quantitative decision-support tool for engineers, enabling more precise mix adjustments based on projected strength outcomes. In practice, the strong correlation between W/C ratio and compressive strength suggests that machine learning-driven optimization can help define the threshold values for water content, ensuring adequate cement hydration while mitigating excess porosity.

The sensitivity of compressive strength to pH fluctuations highlights the necessity of maintaining an optimal alkalinity range when utilizing treated wastewater. This suggests that predictive models can guide engineers in adjusting admixture dosages or introducing pH stabilizers to enhance mix consistency and hydration kinetics. Furthermore, integrating LSBoost predictions into automated mix design workflows allows for real-time strength estimations, reducing reliance on extensive empirical testing. The identification of key predictive variables supports targeted mix modifications, such as the optimized use of supplementary cementitious materials (SCMs), admixtures, and alternative aggregates. By refining material selection and proportioning strategies through predictive analytics, engineers can develop more resource-efficient, high-performance concrete formulations, promoting sustainability while maintaining structural integrity. The robustness of LSBoost in capturing nonlinear interactions further suggests its potential application in adaptive quality control systems, where predictive adjustments can compensate for variability in raw material properties, environmental conditions, or curing regimes. These results highlight the vital role of advanced machine learning methods in improving accuracy, promoting sustainability, and increasing efficiency within contemporary concrete engineering practices.

4 Limitations of the Study

Despite the strong predictive performance of the LSBoost model, several limitations may affect its practical deployment and robustness. The model was trained on literature-based data and lacks validation against field-prepared concrete, highlighting the need for real-world testing. Key environmental factors—such as sulphate exposure, temperature variation, and long-term durability—were not considered, limiting generalization. Additionally, variability in the chemical composition of non-potable water could impact accuracy, suggesting the integration of detailed water quality parameters in future models. Methodologically, the model's sensitivity to data distribution and outliers indicates a need for advanced feature engineering or hybrid AI approaches. Expanding the dataset with site-specific, real-time data will further enhance model adaptability and relevance in sustainable concrete design.

5 Conclusions

This research established a robust machine learning framework aimed at forecasting the compressive strength of sustainable concrete incorporating non-potable water, in response to growing demands for environmental sustainability and resource-efficient practices in construction. An enhanced version of the Least Squares Boosting (LSBoost) model was developed and tested, incorporating statistical evaluation, sensitivity assessment, and explainable AI tools. The model demonstrated excellent performance, achieving a coefficient of determination (R^2) of 0.98 and a root mean squared error (RMSE) of just 1.45, reflecting strong agreement between the experimental and predicted results. These outcomes highlight the potential of intelligent systems to support mix design optimization, minimize material excess, and advance eco-conscious construction methodologies.

One of the notable insights from this investigation is the identification of key input variables influencing compressive strength, including the water–cement ratio, the proportion of fine aggregates, and the pH of the mixing water. Recognizing the significance of these features provides engineers with a practical, data-informed approach to designing concrete mixes, potentially reducing reliance on conventional trial-and-error methods. The study also reinforces the advantages of ensemble learning models in boosting the predictive strength and dependability of AI applications in the domain of civil materials.

While the results are promising, additional research is recommended to confirm the model's effectiveness under real-life construction conditions. Future investigations may explore broader datasets encompassing different treatment levels of non-potable water and evaluate the long-term durability of concrete exposed to diverse environmental factors. Moreover, incorporating more complex AI techniques, such as hybrid deep learning architectures, could further improve predictive accuracy. Advancing these research directions will enhance the role of machine learning in producing high-performance, sustainable concrete solutions that align with environmental goals.

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Credit authorship contribution statement

Sameh Fuqaha: Methodology, Software, Writing – original draft, Reviewing, Formal analysis, and Editing. **Ahmad Zaki:** Data acquisition, Methodology, Supervision, Funding acquisition, Conceptualization, Validation, Reviewing, and Editing. **Slamet Riyadi**: Data acquisition, Investigation, Validation, Methodology, Software, Supervision, Funding acquisition, Conceptualization, Reviewing, and Editing.

Conflicts of Interest

The authors confirm that there are no competing interests related to this study.

Data availability

The datasets, computational models, and source codes used in this research can be obtained by contacting the corresponding author, subject to reasonable request.

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