MACHINE LEARNING-BASED PREDICTION OF COMPRESSIVE STRENGTH OF SELF-COMPACTING CONCRETE INCORPORATING SILICA FUME AND FLY ASH

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ABSTRACT

Self-compacting concrete (SCC) is attracting attention in modern construction due to its excellent flowability, superior consolidation, and suitability for sustainable construction practices. The incorporation of supplementary cementitious materials (SCMs), such as fly ash (FA) and silica fume (SF), improves the mechanical performance and durability of SCC, while reducing cement consumption and minimising environmental impact. Predicting the compressive strength of SCC with various SCMs is challenging due to the nonlinear and interdependent relationships among the mix components. This study investigates the use of machine learning (ML) algorithms to predict the compressive strength of SCC incorporating SF and FA. A database of 400 mixed samples was compiled from previously published articles, which included key mixture parameters such as cement content, water-to-binder ratio, aggregate types, admixtures, and curing age. Five regression-based machine learning models were developed and evaluated: Gradient Boosting Regressor (GBR), eXtreme Gradient Boosting (XGBoost), Random Forest (RF), AdaBoost, and Linear Regression (LR). The evaluation metrics used were R^2, MAE, MSE, and RMSE. Among the models, Gradient Boosting Regression (GBR) achieved the highest predictive accuracy ($R^2 = 0.947$), followed by XGBoost ($R^2 = 0.933$), while Linear Regression showed the lowest accuracy. SHAP and permutation importance analyses revealed that curing age and water-to-binder ratio are the most significant factors influencing SCC strength. The results indicate that machine learning is an effective tool for predicting the mechanical performance of SCC, enabling optimized mix design and reducing experimental efforts in sustainable construction practices.

Keywords: *Machine Learning (ML), Prediction Model, Self Compacting Concrete, Compressive Strength , Fly Ash*

1. INTRODUCTION

Self-compacting concrete (SCC) is a highly flowable, non-segregating concrete that consolidates under its own weight without mechanical vibration (Ahmad et al., 2023; Ismael Jaf, 2023). Its performance is strongly influenced by mix composition, particularly the paste volume and the inclusion of supplementary cementitious materials (SCMs) (Kumar & Rai, 2022). The incorporation of SCMs such as fly ash (FA) and silica fume (SF) enhances both rheological and mechanical properties by improving particle packing, reducing porosity, and strengthening the interfacial transition zone (Leung et al., 2016). Studies have demonstrated that optimal replacements of fly ash (FA) at 20–30% and silica fume (SF) at 5–10% can enhance compressive strength by as much as 25–30%. Additionally, these replacements improve durability against chloride penetration and reduce water absorption (Falmata et al., 2020; Satish et al., 2017). While SCC provides advantages such as lower labor costs, better workability, and enhanced structural performance, its production costs can rise significantly when excessive amounts of cement are used. Therefore, optimising SCC mixtures through SCM incorporation has become an important area of research in sustainable concrete technology.

Compressive strength (CS) is a key indicator of concrete's structural performance, influencing load-bearing capacity, durability, and overall serviceability (Frazão et al.,2015). Reliable prediction of this parameter is essential for ensuring safety, optimising material use, and lessening dependence on extensive, time-consuming laboratory testing. In this context, machine learning offers a sustainable and efficient alternative for accurately predicting concrete strength, which makes it easier to make decisions in concrete design and performance evaluation (Shah et al., 2022).

Recently, machine learning (ML) has emerged as an effective approach for predicting concrete properties, particularly when dealing with complex mixtures containing multiple SCMs or industrial by-products. (Sobuz et al., 2024). ML algorithms can identify nonlinear relationships and hidden interactions among variables, even with limited detailed parameter information (Safayet et al., 2025; Sobuz et al., 2024). Several studies have successfully applied techniques such as Gradient Boosting (GB), extreme gradient boosting (XGBoost), Random Forest (RF), Multi-Linear Regression (MLR), and Linear Regression (LR) models to predict the CS of SCC. For example, (Ismael Jaf, 2023) reported that ANN produced the lowest prediction error when forecasting SCC strength incorporating FA, while (Abdulrahman et al., 2025) demonstrated the strong predictive capability of the Pure quadratic (PQ) model for SCC with various mineral admixtures. Building on these advancements, the present study aims to predict the compressive strength of SCC containing silica fume and fly ash using five advanced ML algorithms: Extreme Gradient Boosting (XGBoost), Random Forest Regressor (RF), Gradient Boosting (GB), AdaBoost, and Linear Regression (LR). The novelty of this study lies in the use of a machine learning model to predict the CS of SCC. The study evaluates all developed models through statistical performance metrics to identify the most accurate predictive approach. Additionally, it determines the key mixture parameters that influence strength development through a permutation importance analysis.

2. METHODOLOGY

Predicting the compressive strength (CS) of self-compacting concrete (SCC) using machine learning (ML) requires extensive datasets containing detailed information about both the mix composition and mechanical performance. The accuracy of any predictive model is highly dependent on the reliability of the input variables. To address this, a comprehensive database was constructed based on a thorough review of previously published studies on SCC that incorporate fly ash (FA) and silica fume (SF). (Aditto et al., 2023; Behfarnia & Farshadfar, 2013; Bingöl & Tohumcu, 2013; Choudhary et al., 2020; Choudhary et al., 2021; E. Güneyisin et al., 2013; Erhan Güneyisi et al., 2015; Krishnapal & Rajeev, 2013; Kumar et al., 2024; Kumar & Rai, 2022; Leung et al., 2016; Sabet et al., 2013; Siddique, 2011; Turk et al, 2013; Wongkeo et al., 2014). The resulting data set contained 400 samples and included nine key input parameters, such as cement content (C)-kg/m³, water-to-binder ratio(w/b), fly ash (FA)-kg/m³, silica fume (SF)- kg/m³, fine aggregate (FnA)-kg/m³, coarse aggregate (CA)-kg/m³, viscosity modified agent (VMA)- kg/m³, Age (Days), and superplasticizer (SP) kg/m³. Outliers and incomplete records were removed following visual and statistical inspections to ensure data consistency. The dataset was then divided into training and testing subsets using a random selection process, with 75% of the data allocated for training and 25% for testing. Statistical analysis and correlation assessments were performed to evaluate data quality, identify trends, and determine the most influential variables affecting the output perimeter in compressive strength (CS) measured in megapascals (MPa).

The study's methodological framework consisted of multiple stages, including exploratory data analysis (EDA), data preparation, model development, model evaluation, and feature interpretation. The EDA phase involved assessing data distribution, identifying variability, and generating a Pearson correlation heatmap to examine linear relationships among variables. Data preprocessing included normalisation and test-train splitting to ensure model generalisation. Multiple machine learning algorithms, LR, AdaBoost, RF, XGBoost, and GB, were developed and optimised through hyperparameter tuning. Model performance was assessed using R^2, MSE, RMSE, and MAE, with the results summarised in a comprehensive comparison table. Feature importance ranking, permutation importance charts, actual versus predicted plots, SHAP summary visualisations, and combined performance metrics graphs were created to improve understanding of model behaviour and identify the most influential variables in predicting SCC compressive strength.

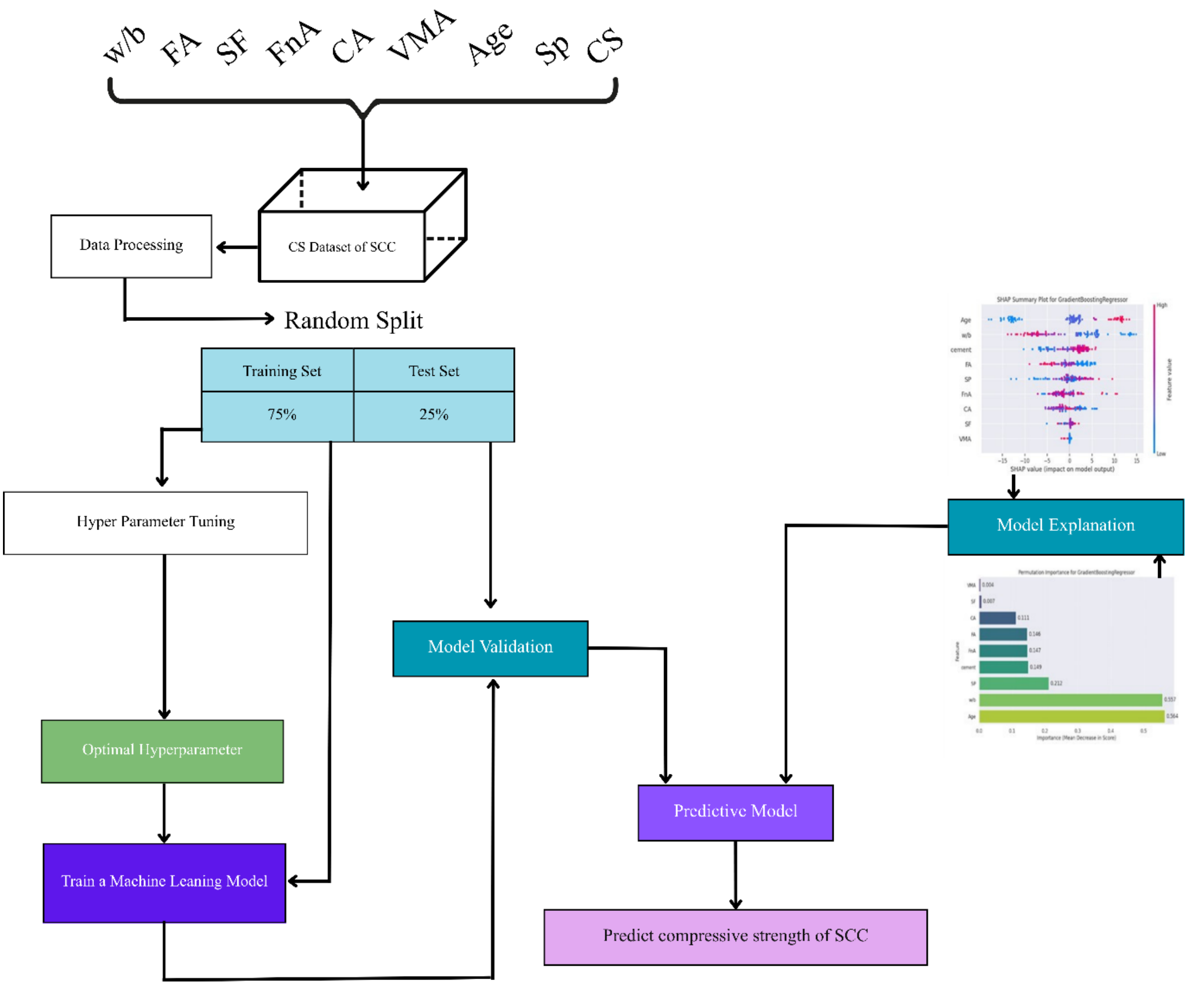


Figure 1: Flowchart diagram for the machine learning approach

Preprocessing

A preliminary preprocessing stage was conducted to enhance the reliability of the SCC dataset. Box-plot analysis in
Figure **2** was employed to examine the distribution of key variables w/b, C, FA, SF, FnA, CA, SP, VMA, Age, and CS. The analysis indicated the presence of significant outliers, particularly in SF, VMA, and Age, which could deform the data's statistical structure. To address this, outliers were removed using interquartile range based thresholds, resulting in a more consistent and representative dataset. Subsequently, all variables were normalised to a common scale to prevent excessive influence from defferences in measurements unit. These preprocessing steps enhanced data consistency and ensured more reliable performance in the following correlation assessment and model development stages.

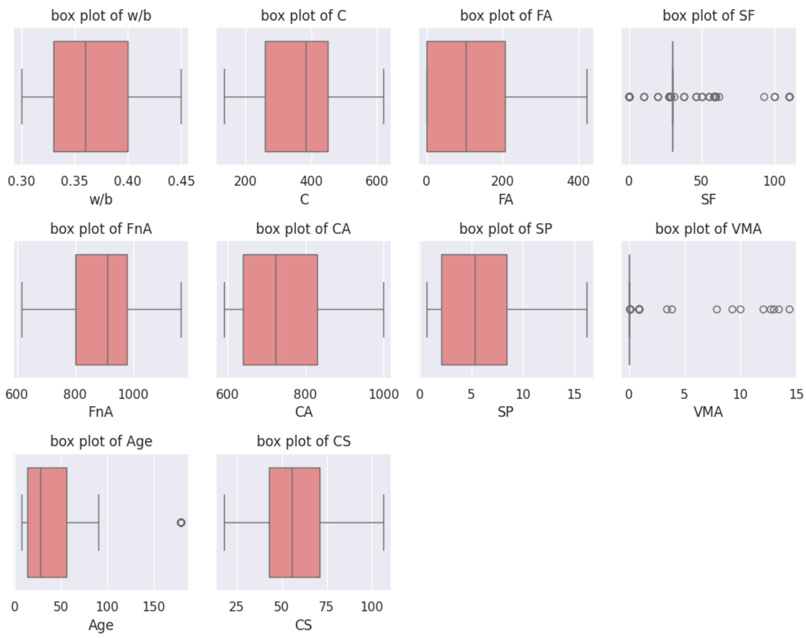


Figure 2: A box plot for all dependent and independent parameters of SCC

Statistical Evaluation

The collected data were analysed statistically to identify the distribution patterns of each independent variable concerning the dependent variable, CS. This method produces statistics for data frame columns, summarising the central tendency, dispersion, and distributional shape for each numerical column. The output includes count, mean, standard deviation, minimum and maximum values, and the interquartile range (25th, 50th, and 75th percentiles). Understanding the basic characteristics of a dataset is a useful initial step in EDA. A summary of the computed statistical parameters is provided in the table Table 1.

Table 1: Summary of statistical analysis for all parameters of the dataset

	w/b	**C**	**FA**	**SF**	**FnA**	**CA**	**SP**	**VMA**	**Age**	**CS**
count	414	414	414	414	414	414	414	414	414	414
mean	0.37	366.2	120.9	30.4	904.4	736.7	5.7	0.26	41.5	56.6
std	0.05	119.7	119.8	16.1	120.8	112.3	3.9	1.6	38.8	18.3
min	0.3	135	0	0	614.3	590	0.6	0	7	17.7
25%	0.33	259	0	30	801	640	2.1	0	14	43
50%	0.36	382.5	103	30	910	722	5.3	0	28	55.4
75%	0.4	450	206	30	980	829	8.4	0	56	70.9

max	0.45	620	420	110	1166	1000	16.2	14.33	180	106.6

Models Theory

Linear Regression (LR)

Linear Regression (LR) is the simplest supervised learning model used to establish a linear relationship between input features and a target variable. It is a foundational machine learning approach that predicts a continuous target variable by creating this linear relationship between the input data and the output. To fit a line to the data, LR minimizes the sum of squared residuals, which is the difference between the observed values and the predicted values. However, because it assumes a linear relationship between the variables, LR may not perform well when dealing with non-linear data.

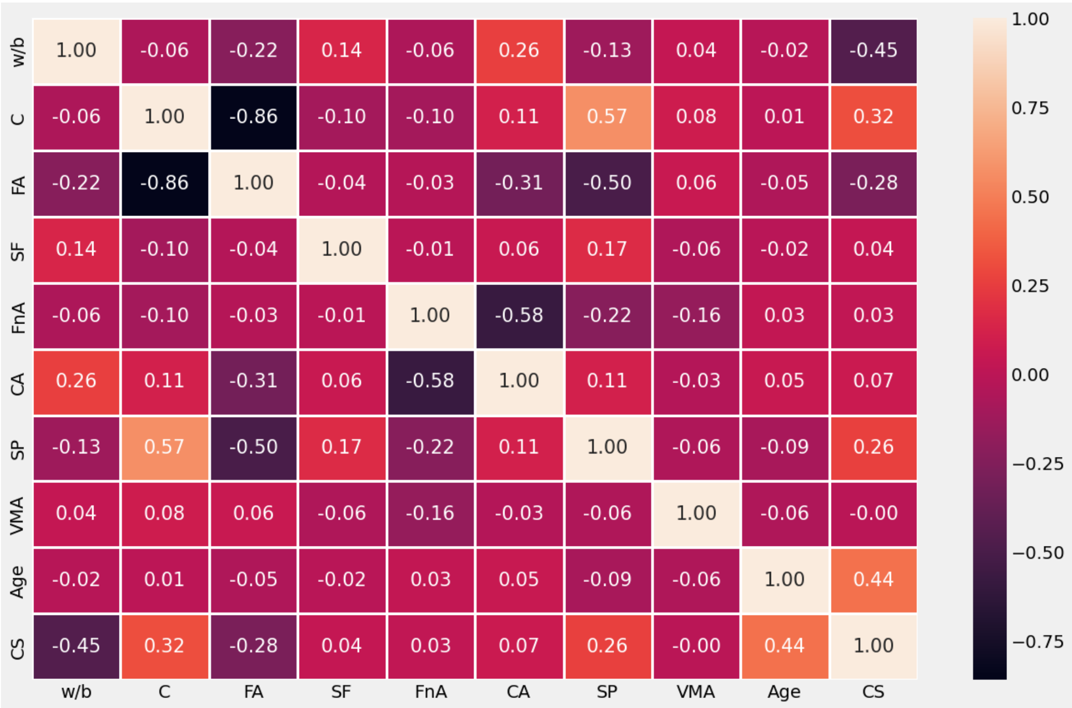


Figure 3: The Pearson correlation coefficient between all dependent and independent variables.

AdaBoost

AdaBoost is an ensemble learning algorithm that builds a strong predictive model by sequentially combining multiple weak learners, usually shallow decision trees. In each iteration, the algorithm increases the weights of samples that were misclassified, encouraging subsequent learners to focus more on these challenging cases. The final prediction is made by aggregating the outputs of all the learners, with those that are more accurate having a greater influence on the overall prediction.

Random Forest Regressor (RF)

Random Forest (RF) is an ensemble learning algorithm that combines predictions from multiple decision trees to enhance both validity and accuracy. Each tree is trained on a bootstrap sample of the dataset, and a random subset of features is considered at each node split. The final prediction of the ensemble is calculated by averaging the individual predictions from the trees.

Extreme Gradient Boosting (XGBoost)

Extreme Gradient Boosting (XGBoost) is an advanced boosting algorithm that constructs an ensemble of weak learners (decision trees) sequentially, where each new tree corrects the residual errors of previous trees. The model minimizes a regularized objective function (Chen & Carlos Guestrin,2016).

Gradient Boosting (GB)

GB is an advanced ensemble learning approach that incrementally improves prediction accuracy by constructing successive decision trees that correct the residual errors of preceding models (Natekin & Knoll, 2013). By iteratively minimising a specified loss function using gradient descent, GB effectively integrates multiple weak learners into a robust predictive model suitable for both regression and classification applications (Pal et al., 2025). In this study, the GB model was trained using a learning rate of 0.2, a squared-error loss function, and 160 estimators.

Measures to Evaluate Developed Models

Various statistical indicators are commonly used to evaluate the performance of machine learning models. This study, however, focused on four widely recognised metrics, such as Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Mean Square Error (MSE), and the Pearson correlation coefficient (R^2). MAE represents the average of the absolute differences between the predicted values and the actual values (Kang et al., 2021).

Table 2: Equation and allowable ranges for statistical indicators

Equation	Acceptable range	References
$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y})^2}$	Close to 1	(Dong et al., 2022)
$RMSE = \sqrt{MSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$	MAE < RMSE	(Iqbal et al., 2021)
$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$	Closer to zero (0≤MSE≤∞)	(M, 2021)
$MAE = \frac{1}{N}\sum_{i=1}^{N}\lvert y_i - \hat{y}_i\rvert$	Greater than 0.65 for an excellent model	(N. Moriasi et al., 2007)

Mean Squared Error (MSE) quantifies how far the predicted values deviate from the actual observed values by calculating the average of the squared differences between them. Due to the squaring process, MSE gives greater weight to larger errors, penalising them more heavily. Represents the standard deviation of the prediction errors and places greater emphasis on larger deviations. A lower RMSE value signifies higher model accuracy, making it a useful indicator of predictive performance (Kang et al., 2021). In regression analysis, the coefficient of determination (R^2) quantifies the proportion of variance in the dependent variable explained by the independent variables. The R^2 value is calculated by comparing the variance of the observed data with that of the predicted data, with higher R^2 values reflecting a better model fit (Feng et al., 2020).

3. RESULTS AND DISCUSSIONS

Several ML algorithms were employed to predict the CS of self-compacting concrete (SCC). Model performance was assessed by comparing predicted values with experimental results, and the feature importance of the four best-performing algorithms was examined to ensure the robustness and interpretability of their predictions. Evaluation metrics such as MAE, MSE, RMSE, and R^2 were used to compare model accuracy. Lower MAE, MSE, and RMSE values reflect improved predictive precision, whereas higher R^2 values indicate stronger agreement between predicted and measured compressive strengths. Collectively, these indicators provide a comprehensive basis for selecting the most suitable model for estimating the compressive strength of SCC.

Table 3: Accuracy score and errors for all models

Model	MSE	RMSE	MAE	R^2
GBR	15.448	3.93	3.05	0.947
XGBoost	19.597	4.427	3.286	0.933
RF	35.30	5.94	4.09	0.880
Adaboost	89.84	9.48	7.96	0.694
LR	174.67	13.22	10.70	0.405

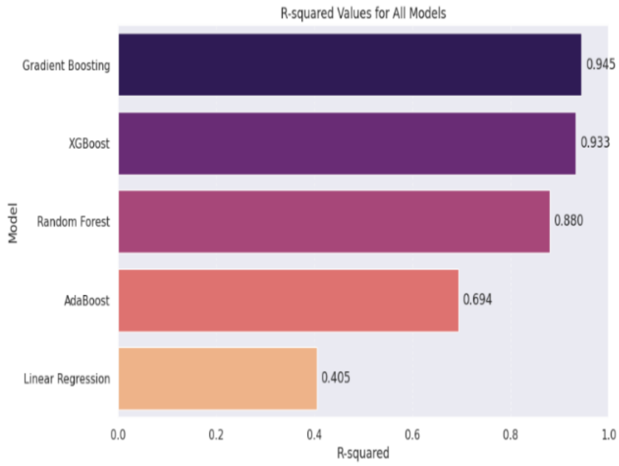


Figure 4: Bar plot for coefficient of determination for all models

Table 3 presents the performance of the regression models evaluated in this study, further demonstrating the strong capability of these techniques to predict the compressive strength of SCC. As illustrated in Figure 4, The Gradient Boosting Regressor (GBR) showed better predictive accuracy than other analyzed ML models.

Figure 4 summarises the R^2 values of all regression models, providing a clear comparison of their predictive performance. GBR achieved the highest accuracy, with an R^2 of 0.945, closely followed by XGBoost, with an R^2 of 0.933. The Random Forest (RF) model achieved an accuracy of 0.880. In contrast, AdaBoost and Linear Regression (LR) showed significantly weaker predictive capabilities, with R^2 values of 0.694 and 0.405, respectively. These results confirm previous findings that boosting-based ensemble models, particularly Gradient Boosting Regression (GBR), offer enhanced accuracy in estimating the compressive strength of self-compacting concrete SCC.

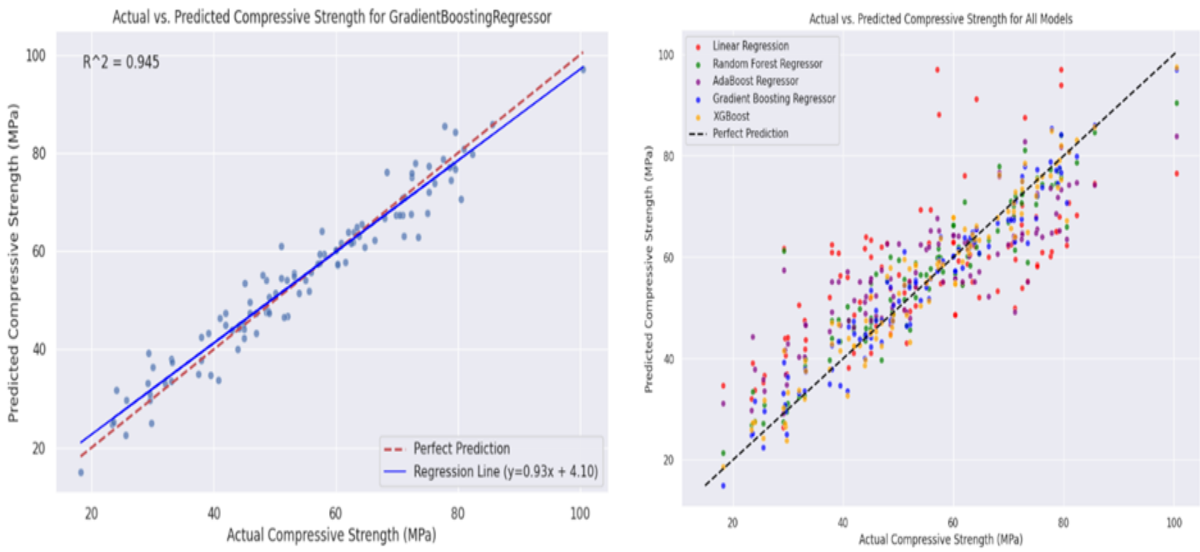
The actual versus predicted plots in

Figure 5(a) and

Figure 5(b) provide a clear visual representation of the predictive capability of the machine learning models used for estimating the CS of SCC.

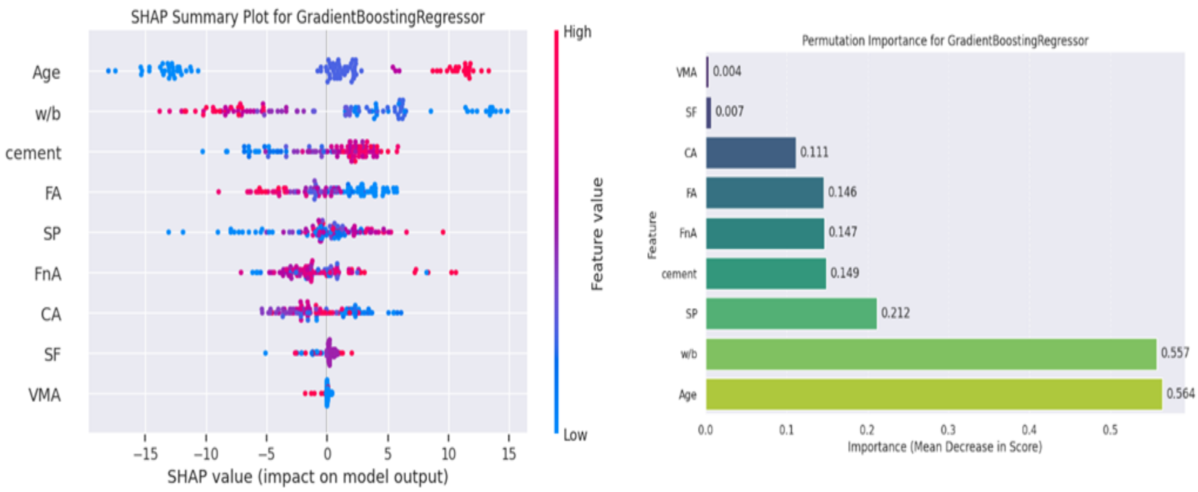
Figure 5(a),highlights the Gradient Boosting Regressor (GBR) and illustrates a strong linear relationship between the predicted and measured compressive strength (CS). The model shows minimal dispersion around the regression line and achieves a high coefficient of determination (R^2 = 0.945). This shows that the GBR accurately captures the nonlinear behaviour influencing the development of SCC strength.

Figure 5(b) compares the performance of all the regression models used in this study. Each model demonstrates a positive correlation between actual and predicted values. However, there are notable differences in predictive precision. The GBR and XGBoost models exhibit the closest clustering of points along the 1:1 reference line, which aligns with their superior quantitative performance (R^2 = 0.947 and 0.933, respectively). In contrast, the RF model shows moderate alignment with the reference line, but with noticeably greater scatter, indicating lower predictive accuracy. Both AdaBoost and Linear Regression show significant deviations from the ideal prediction line, which reflects their higher error metrics and weaker explanatory power.



(a) (b)

Figure 5: Plot for (a) GradientBoosting Regressor : Predected against actual (b) all models : Predected against actual

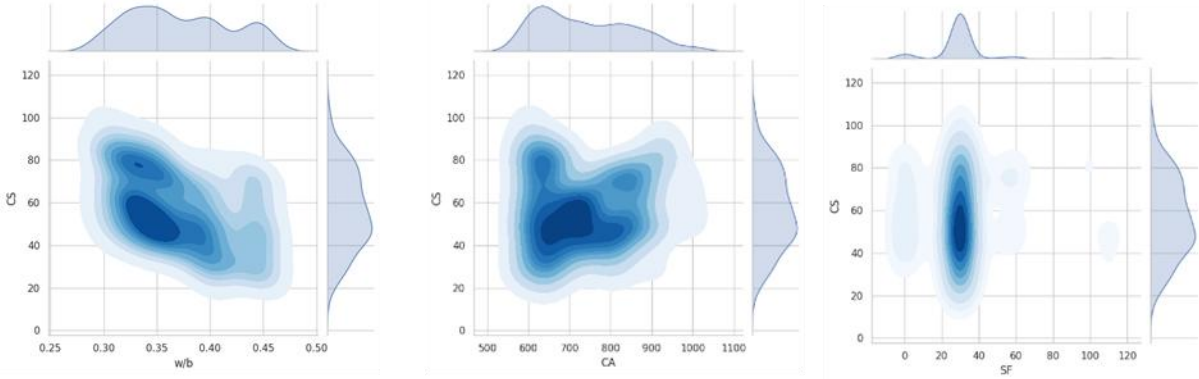


(a) (b)

Figure 6: Plot for gradient boosting regressor (a) SHAP bees-warm Feature impact, (b) Permutation importance for

Effect of SHAP Value on Model Output

Figure 6(a) illustrates the results of the SHAP analysis, which shows the relative influence of each input parameter on the predicted CS of self-compacting concrete. Among all the features, age is identified as the most significant factor, demonstrating a strong positive effect on strength development. The w/b has a notable negative impact, as higher values consistently reduce compressive strength, consistent with established concrete behaviour. Cement content positively affects strength, underscoring its vital role in the formation of compressive strength. FA and SP have a moderate influence, with their effects varying based on specific mix proportions. Other parameters, such as FnA, CA, SF, and VMA, show comparatively lower influences, although their trends are consistent with SCC mix design. Overall, the SHAP plot provides a clear, transparent interpretation of feature contributions, validating the model's behaviour.

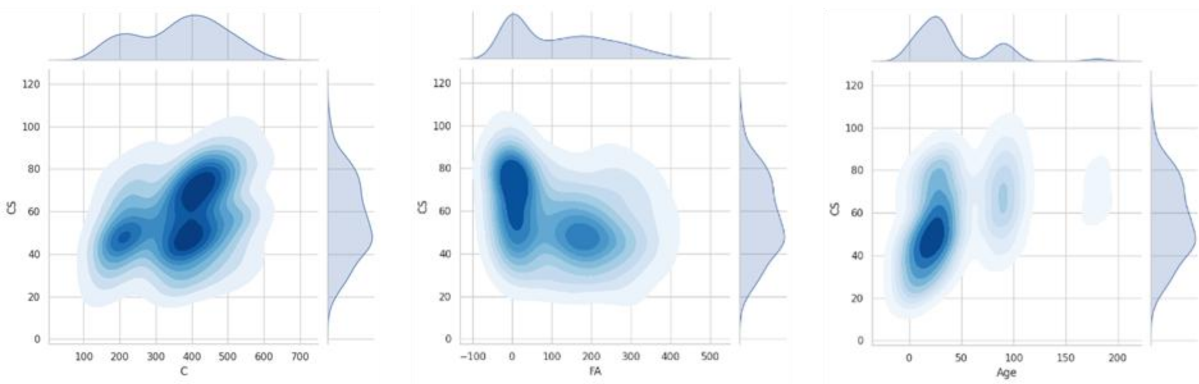


(a) (b) (c)

Figure 7: Distribution of input parameters and relationship with compressive strength

Effect of Permutation Importance on Model Output

Figure 6(b) illustrates the results of the permutation importance analysis, which highlights the relative contributions of each input feature to the predictive performance of the Gradient Boosting Regression (GBR) model used to estimate the compressive strength of SCC. The analysis indicates that Age and the w/b are the two most influential variables. These features exhibit the most significant decreases in model performance when permuted, with importance values of 0.564 and 0.557, respectively. This underscores their dominant roles in strength development and overall mix performance. Additionally, the SP content and cement content also show considerable influence, highlighting their critical roles in the SCC.



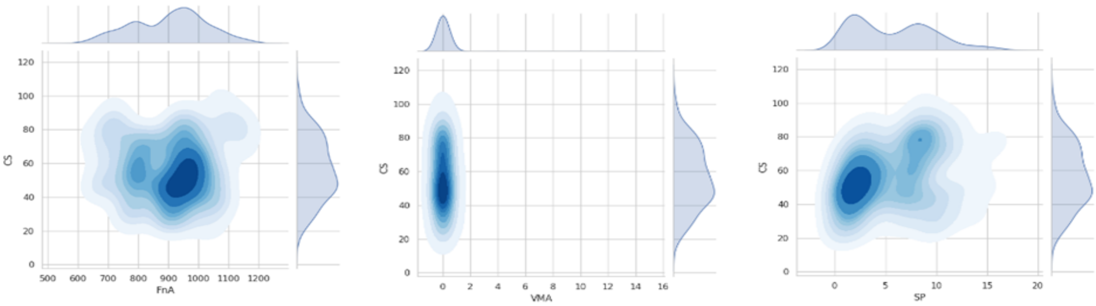
(d) (e) (f)

Figure 7: (continued)

Conversely, features such as silica SF and the VMA contribute minimally to prediction accuracy, reflecting their relatively smaller influence within the dataset. Overall, the permutation importance plot validates the model's behaviour and aligns well with established material science principles governing SCC performance.

Dataset Distribution and Correlation between Features

The correlation coefficients between each variable were calculated and are shown in Figure 3. A correlation matrix, a statistical technique used to assess the direction and strength of relationships among variables, was employed to analyse the associations between the dependent and independent variables. This analysis offered valuable insights into how different parameters are interrelated, the correlation coefficient ranges between -1 and +1, where the sign indicates whether the relationship is positive or negative. Figure 3 depicts the correlation patterns between the independent and dependent variables. A notable negative correlation was found between compressive strength (CS) and w/b and FA, with a correlation coefficient of approximately –0.45 and -0.28, respectively. In contrast, compressive



(g) (h) (i)

Figure 7: (continued)

strength exhibited a positive relationship with curing time, reflected by a coefficient of 0.558. Additionally, a strong negative correlation was observed between cement content and the w/b, with a coefficient of –0.744. The correlation coefficients between compressive strength and other independent variables were 0.32, 0.04, 0.03, 0.07, 0.26, and 0.44 for C, SF, FnA, CA, SP, and Age respectively.

Figure 7 illustrates the distribution of primary input parameters and their associations with CS. The contour plots clearly show that cement content has a strong positive relationship with strength, with the most significant gains occurring between approximately 350 and 500 kg/m³. Fine aggregate also has a favorable influence on strength within the range of 600 to 1200 kg/m³, while coarse aggregate shows a moderate correlation around 700 to 1100 kg/m³. The VMA has minimal impact across its observed range, indicating that strength is not particularly sensitive to this parameter. Additionally, the dosage of superplasticize positively affects strength development, especially between 5 and 10 kg/m³. Conversely, higher water-to-binder ratios are associated with reduced strength, which aligns with expectations. Curing age exhibits a strong progressive correlation with strength, with notable increases observed during the initial hydration period, particularly up to 56 days. These visual distributions collectively highlight the key parameter ranges that most significantly influence the strength performance of self-compacting concrete, providing essential guidance for optimizing mix design.

4. PRACTICAL IMPLIMENTATION

The findings of this study offer significant practical value to the construction industry, especially in promoting sustainable concrete production. The developed machine learning models provide an efficient way to predict the mechanical performance of SCC that incorporates FA and SF. These models enable engineers to quickly assess different mix scenarios and optimize the balance between strength and sustainability without conducting extensive laboratory tests. Furthermore, the results emphasize the increasing demand for user-friendly engineering tools or software that can directly estimate concrete strength, providing a practical interface for industry applications.

5. CONCLUSIONS

This study demonstrates the effectiveness of ML techniques in predicting the CS of self-compacting concrete that incorporates SF and FA. Among the five regression models evaluated, the GBR exhibited the highest predictive accuracy, followed closely by XGBoost. In contrast, the RF model showed moderate performance, while AdaBoost and LR performed significantly worse. This highlights the superiority of boosting based ensemble methods for modelling the strength of SCC. Feature interpretability analyses indicated that curing age and w/b were the most influential variables across all models. Additionally, the results from SHAP and permutation importance further confirmed the significant roles of binder composition, and mixture proportions in determining compressive strength. The developed models not only enhance understanding of the underlying parameter contributions but also provide a practical, cost-effective tool for optimising SCC mix designs. By reducing the need for extensive laboratory testing, these predictive frameworks support more sustainable concrete production and facilitate decision making in engineering practice. Future work may extend these models using larger datasets, hybrid ML architectures, and software integration to improve prediction accuracy and further practical accessibility.

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