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PREDICTING THE COMPRESSIVE AND FLEXURAL STRENGTH OF ULTRA-HIGH-PERFORMANCE CONCRETE USING MACHINE LEARNING MODELS

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ABSTRACT

Ultra-high-performance concrete (UHPC) is a cutting-edge construction material by its superior mechanical properties and durability. In modern times, the application of machine learning (ML) approaches has been popular and helpful in accurately predicting the strength properties of UHPC. Additionally, these methods have been vital in analysing and identifying the key input parameters necessary for creating an optimal mix design. There is an existing research gap in the prediction modelling of the UHPC for both compressive strength (CS) and flexural strength (FS) using machine learning. Additionally, the strength of UHPC depends on multiple input parameters and materials. In this study, machine learning models such as adaptive boosting (AdaBoost), random forest regression (RFR), and extreme gradient boosting (XGBoost) with grid search for hyperparameter tuning were used to predict the compressive and flexural strength of UHPC. The results showed that XGBoost model was the most accurate in predicting the CS (R^2 0.93) and flexural strength (R^2 0.90) of UHPC, according to comparisons of the AdaBoost and RF models. For the novel method, Shapley Additive Explanations (SHAP) was used to provide explanations for the XGBoost model and to understand the influence of input parameters on the compressive and flexural strength. Shapley Additive Explanations (SHAP) analysis showed that the age and steel fiber had the greatest influence on the CS and FS strength of UHPC. The overall outcome of this research will aid in designing an optimum mix design along with suitable materials usage, which will reduce extra labor, lab tests, material usage, and time consumption.

INTRODUCTION

Concrete is one of the most extensively utilized materials in the modern world, playing a significant role in infrastructure development. It has a major negative impact on the environment, contributing to 7% of worldwide carbon dioxide emissions(Alabduljabbar et al., 2023). The modern construction industry's evolving demands have outgrown conventional concrete, creating a necessity for high-performance concrete materials (Wijesundara et al., 2025). Ultra-High-Performance Concrete (UHPC) is an advanced cementitious material that has been in high demand in the construction industry over the last decade. UHPC has excellent mechanical properties characterized by compressive strength of at least 120 MPa, a tensile strength greater than 7 MPa, high ductility, remarkable durability, and toughness (Jiao et al., 2022; Katlav and Ergen, 2025). It generally consists of steel fibers, sand, silica fume, ordinary Portland cement (OPC), and high-range water-reducing additives. It has highly effective advantages, such as high-rise buildings, lighter dead weight-load structures, long-span bridges, tunnels, marine structures, and precast elements (Alabduljabbar et al., 2023). Therefore, the structure provides high durability, a long service life, and minimal maintenance requirements.

In recent years, researchers have been attracted to applying machine learning methods in civil engineering for predicting material mechanical strength, material performance, structural engineering optimization, structural health monitoring, and mix proportion optimization (Zhang et al., 2024). Machine Learning (ML) model provides a promising alternative to traditional experimental approaches. Accurately predicting the mechanical properties is crucial in structural engineering for innovative UHPC materials (Li et al., 2024). Predicting the mechanical properties of UHPC, including compressive and tensile strength, is challenging because of its different types of material composition. The foremost difficulty is ensuring the input data or concrete mix design data, which directly impact prediction accuracy. Generally, UHPC is made up of different materials, such as cement, silica fume, aggregates, fibers, water, fly ash, superplasticizers, supplementary cementitious materials, and filler materials (Alabduljabbar et al., 2023). However, finding the optimum mixture for UHPC sampling is difficult and lengthy. As a result, machine learning approaches have replaced experimental work in forecasting the mechanical properties of UHPC (Gong and Zhang, 2023).

Nowadays, machine learning techniques have been employed to predict the mechanical characteristics of concrete, including its tensile strength, flexural strength, compressive strength, durability, cracking behavior, and structural performance. Several studies have applied regression models, neural networks, machine learning algorithms, and ensemble methods to predict the performance of concrete mixes(Gong and Zhang, 2023; Wakjira et al., 2024; Zhou et al., 2023). According to Li et al. 2024, ML methods demonstrated good prediction accuracy for the compressive strength of UHPC, using three meta-heuristic optimization algorithms used (Li et al., 2024). A recent study by Wijesundara et al. (2025) found that the XGBR model demonstrated high accuracy, achieving an R^2 value of 0.905, among other machine learning models for predicting the compressive strength of UHPFRC. Additionally, the study provided SHAP analysis for more detailed interpretations (Wijesundara et al., 2025). Xi et al., developed a machine learning model to predict the self-healing performance of Ultra High-Performance Concrete (UHPC) using meta-heuristic algorithms, and models prediction performance R^2 over 0.92 for training stage and more than 0.85 for testing stage for each optimization ML algorithms (Xi et al., 2023). Aylas-Paredes et al. proposed using machine learning models to predict the compressive strength of UHPC based on a comprehensive database of 1,300 data records. SHAP analysis revealed that while chemical compositions influence the predictions, their impact is relatively minor compared to other factors (Aylas-Paredes et al., 2025).

Emad et al. proposed soft computing techniques, such as nonlinear relationship (NLR), pure quadratic, M5P-tree (M5P), and artificial neural network (ANN) models, to predict the compressive strength of UHPFRC, with the ANN model demonstrating the best performance among the other machine learning models (Emad et al., 2022). Kumar et al. used deep neural networks and ensemble machine learning algorithms, including gradient boosting, extreme gradient boosting, random forest regressor, extra tree regressor, and voting regressor, trained on a dataset of 810 UHPC mixture samples with 15 input variables to predict the compressive strength of UHPC, with the extra tree regressor achieving the highest accuracy among all models (Kumar et al., 2023). Another study explored a dataset of 810 records collected for predicting the compressive strength of UHPC, utilizing gene expression programming (GEP) and SHAP analysis. The findings indicate that the GEP model demonstrated superior accuracy, achieving an R value of 0.98. Additionally, age, silica fume, and fiber had a positive impact on compressive strength (Alabduljabbar et al., 2023). Despite the utilization of machine-learning algorithms, the use of UHPC is still in its early stages. This study aims to bridge this gap by employing machine learning models (ML), including XG-Boost, Ada-Boost, and Random Forest, to optimize the mechanical strength of UHPC composites. Few studies have been published on predicting the compressive and flexural strength of UHPC, as well as investigating the impact of mix design parameters using SHAP analysis. Therefore, the research objectives are as follows: (1) develop machine learning models for predicting compressive strength (CS)

and flexural strength (FS), (2) compare the prediction performance to identify the best model, and (3) utilize the novel SHAP method to analyze the impact of input variables on CS and FS prediction.

MATERIALS AND METHODOLOGY

DATA SOURCES AND STRUCTURES

In this research utilized data collected from literature to predictions using well-established machine learning models (https://data.mendeley.com/datasets/dd62d5hyzr/1). The compressive and flexural strength values of the mixes used in UHPC sample were determined based on data from published article (Mahjoubi et al., 2023, 2022). The primary focus of this study was to predict the Compressive (CS), and Flexural (FS) strengths of UHPC. The models utilized 17 input variables including Cement content (cement), Fly Ash (FA), Slag content (slag), Silica fume (SF), Nano silica (NS), Limestone powder (LSP), Sand content (Sand), Coarse Aggregate (CA), Water content (Water), Superplasticizers (SP), Polystyrene fiber (PF), Polystyrene fiber diameter (PFD), Polystyrene fiber length (PFL), Steel fiber (SF), Steel fiber diameter (SFD), Steel fiber length (SFL), and Curing time (Age). A dataset comprising 630 data points was employed to analyse compressive strength, and the 315 of data points was used to predicting flexural strength. In this study, two phases were used for the proposed machine learning model: training and testing phases. The training phase used randomly 70% of the datasets, and remaining 30% were used to testing and phases. Throughout the analysis, both sets were iteratively employed for training and testing, aiming to construct accurate predictive models that closely aligned with the experimental observations of the output variables.

MACHINE LEARNING MODELS

The present study employed three machine learning (ML) algorithms, such as AdaBoost regression (AB), Random Forest regression (RF), and Extreme Gradient Boost regression (XGBoost), with optimization using grid search to forecast the mechanical properties. The machine learning analysis was conducted using the Python programming environment within the Jupyter Notebook. The dataset was randomly split into 70% for training and 30% for testing to ensure robust model evaluation.

ADABOOST REGRESSION (AB)

AdaBoost is an ensemble method developed by Yoav Freund and Robert Schapire in 2003 for performing statistical classification tasks(Rathakrishnan et al., 2022). Boosting techniques are frequently used in supervised machine learning to decrease variation and bias. The weak learner gets improved by ensemble methods(Freund and Schapire, 1997). AdaBoost is an iterative approach which modifications the weights of the weak learners in every round until the specified error is achieved. During the iteration phase, samples with incorrect predictions in the previous round are assigned higher weights, while those with accurate predictions receive lower weights. The final prediction is determined by aggregating the weighted votes of the weak learners(Min et al., 2023).

RANDOM FOREST REGRESSION (RF)

Random Forest is an effective regression approach developed in 2001 by Leo Breiman and Cutler Adele (Khan et al., 2025). The RF technique is a combined approach that uses bagging and decision tree methods(Li et al., 2024). RF model is an advanced version of DTR method which employs multiple decision trees trained on different subsets of the data sample. The RF model consists of leaf nodes, root

nodes, and branches. The observed data is represented by a tree's root, and a potential choice is shown by its branches. The output of the algorithm is represented by the tree's leaves. This method rapidly relates the input and outcome characteristics, providing precise forecasts in a shorter time frame(Wijesundara et al., 2025).

EXTREME GRADIENT BOOST REGRESSION (XGBOOST)

XGBoost is an effective machine learning model for regression applications that based on the gradient boosting decision tree approach. XGBoost is an ensemble learning technique that employs gradient boosting to combine the predictions of multiple weak learners, typically decision trees, into a robust and accurate final prediction (Sibindi et al., 2023). XGB is a versatile and powerful machine learning algorithm that excels in predictive accuracy, handling structured data, and avoiding overfitting. This model builds trees in parallel, whereas GBR does it sequentially. This significantly improves computing efficiency for XGBoost model (Guo et al., 2023). Most important, regular GBR models lack regularization, which can lead to overfitting. XGBoost employs sophisticated regularization approaches, including pruning and regularization terms, which help reduce overfitting and improve modelling generalization (Wijesundara et al., 2025).

SHAP

Lundberg and Lee proposed utilizing SHAP to elucidate machine learning forecasts based on the concept of games (Lundberg et al., n.d.). For instance, the prediction becomes the payment, and the inputs are identified as participants. This method allows for the interpretation of individual input features' impact on the predicted output, making it especially valuable for explaining complex models. The SHAP technique, rooted in game theory, assumes that each feature in the input data contributes to the model's prediction. The contribution of each feature is quantified using its Shapley value, which measures its importance relative to other features in the model(Ekanayake et al., 2022). This approach offers a structured framework for understanding feature influence on the output and has been proven effective in explaining the behavior of complex machine learning models.

PERFORMANCE METRICS

In this study, the performance of the developed ML models is assessed using four metrics: the coefficient of determination (R^2), root mean squared error (RMSE), mean square error (MSE), and mean absolute percentage error (MAPE). Machine learning models is more accurate if the R^2 value (1 is the ideal value) and the error values (RMSE, MAPE, and MAE) are small (0 is the ideal value).

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(O_i - P_i)^2}{\sum_{i=1}^{n}(O_i - \mu_i)^2} \quad (1)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(O_i - P_i)^2} \quad (2)$$

$$MAE = \frac{\sum_{i=1}^{n}|P_i - O_i|}{n} \quad (3)$$

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\left|\frac{O_i - P_i}{O_i}\right| \quad (4)$$

Where O_i represents actual value, P_i denotes predicted value, μ_i bar is the mean, $\bar{O}_i$ represents the average of observation values n is the total values in the sample.

RESULTS AND DISCUSSION

Figs. 1 and 2 displayed the predicted results of compressive strength and flexural strength using the three machine learning models such as XGBoost, RFR, and AdaBoost—at both stages, along with the dataset accuracy. To verify their data adjustments, the predicted and observed datasets were combined. The datasets below show the error of the predicted and observed datasets obtained through FS and CS. It is notable that the XGBoost model is well adjusted for the real and predicted datasets at both phases. It also displays the very few error ranges during the train and test stages for flexural and compressive strength in Figs. 1 and 2. The XGBoost model exhibits the error range around from -0.5 to +0.5 and -10 to +10 MPa during train and test stages, respectively, for CS and also shows that from -0.5 to +0.5 and -4 to +4 at the train and test stages, respectively, for FS. However, the AdaBoost models represented the error range of about between -25 and +25 at both the train and test phases for CS. It is also noticeable that the AdaBoost model found an error range from -10 to +10 MPa for FS, which is more than the XGBoost model. In addition, the RF model displays moderately adjusted actual and predicted data points, and the error range is less than AdaBoost but more than XGBoost. Overall, The XGBoost model performs better than other models.

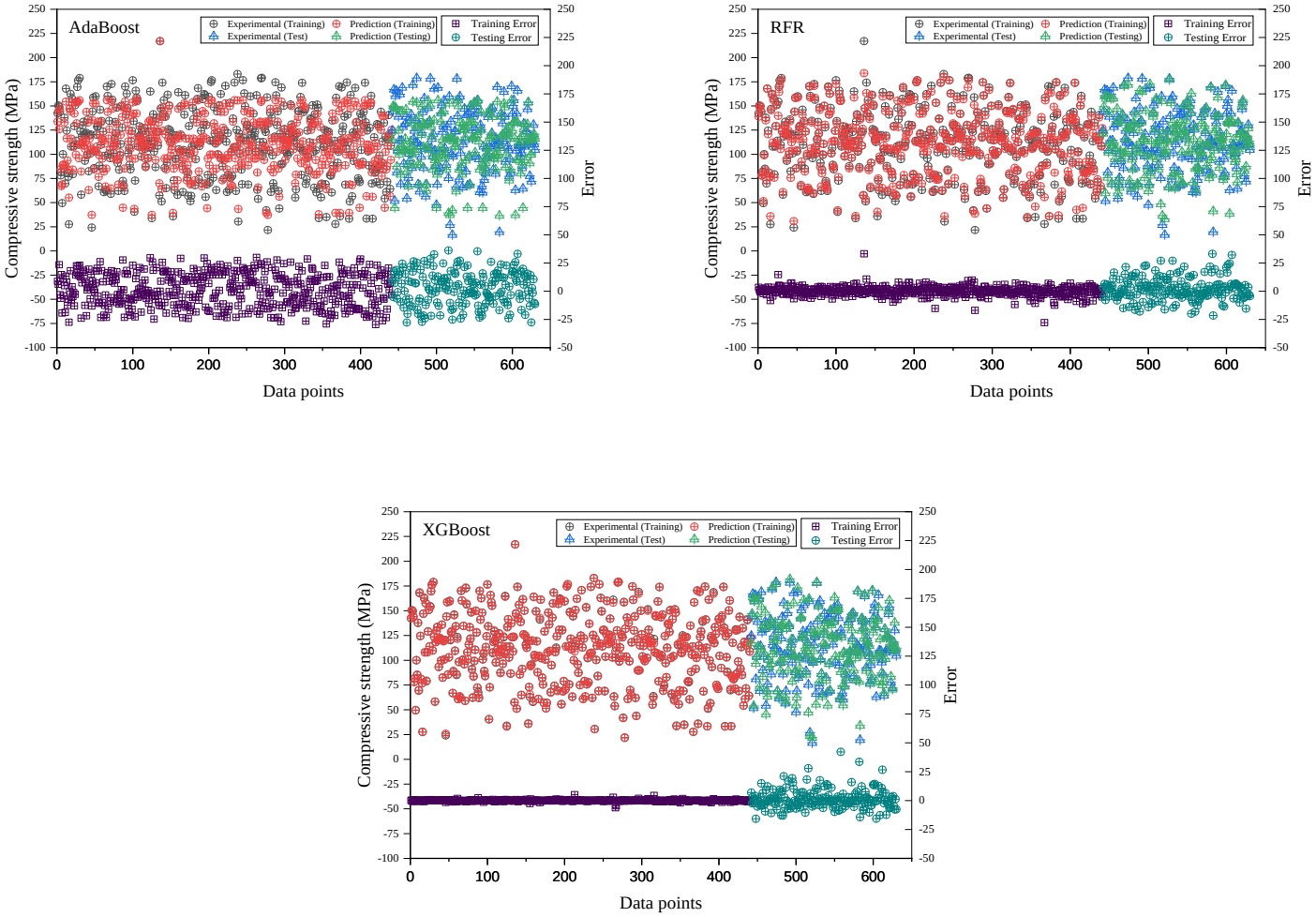

Figure 1. Observed vs predicted values trend with error analysis of CS.

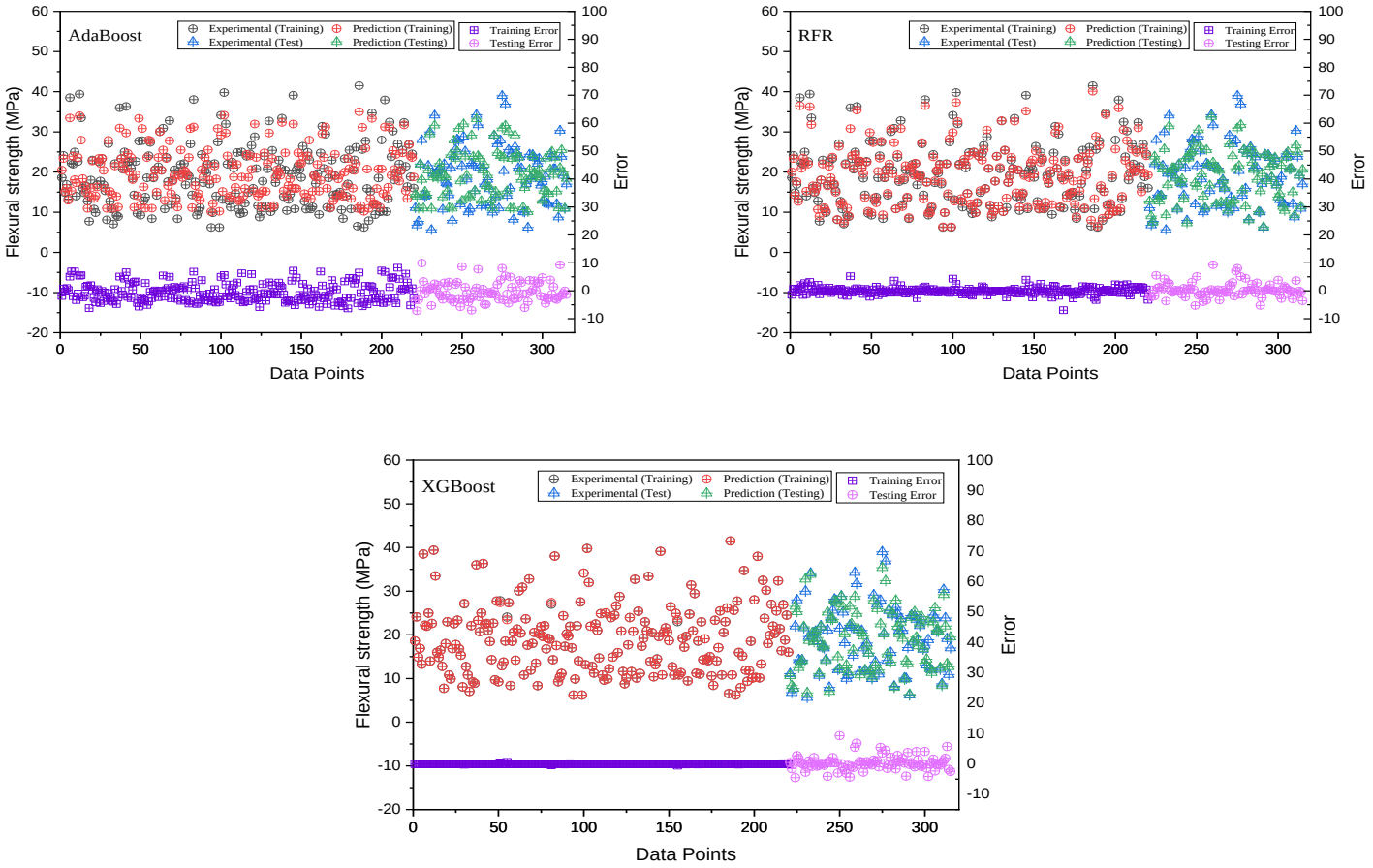

Figure 2. Observed vs predicted values trend with error analysis of FS.

Table 1 demonstration that evaluation metrics for three machine learning models (AdaBoost, RFR and XGBoost). The actual and predicted data were taken into consideration for analysing the results of the goodness of fit limits, including R^2, RMSE, MAE, and MAPE. XGBoost model R^2 value was found to be about 0.9992 and 0.9343 at the train and test stages, respectively. The XGBoost model shows a high R^2 value, which indicates good accuracy for CS prediction. The RF and AdaBoost models R^2 value was found to be 0.9851 and 0.8302 at the train stage, respectively. The RMSE values of the XGBoost, RF and AdaBoost models show around 8.343, 10.388, and 15.208 during train stage, respectively. The XGBoost model provides a lower RMSE value and AdaBoost provides a higher RMSE value. In addition, the MAE value displays almost 5.640, 7.843 and 12.796 at the testing stage, the XGBoost, RF and AdaBoost, respectively. Moreover, almost 0.62%, 3.49% and 13.23% of the MAPE value were found from XGBoost, RF and AdaBoost at the training stage, respectively. Table 1, for FS, the R^2 value was found in the XGBoost model around 0.999 and 0.897 during the training and testing stages. The AdaBoost and RFR models show R^2 values of 0.7642 and 0.8772, respectively, during the test phase. In addition, at the train and test stages, the RMSE values of 0.063 and 2.312 of the XGBoost models, respectively. The AdaBoost and RFR models were found to be 3.4994 and 2.525 at the test phase, respectively. Moreover, most noticeably, the XGBoost model displays the MAE and MAPE values lower than the AdaBoost and RFR at both phases. Overall, the XGBoost model has better performance than the AdaBoost and RFR models because the XGBoost model provides good value for statistical evaluation parameters.

Table 1 Performance comparison of the different models

Models Predict CS	Training				Testing			
	R^2	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE
AdaBoost	0.83	14.63	12.61	13.22%	0.78	15.21	12.8	13.07
RF	0.98	4.32	2.95	3.49%	0.90	10.39	7.84	8.30
XGB	0.99	0.98	0.61	0.62%	0.93	8.34	5.64	5.79%

Models Predict FS	Training				Testing			
	R^2	RMSE	MAE	MAPE	R^2	RMSE	MAE	MAPE
AdaBoost	0.81	3.41	2.86	17.98%	0.76	3.49	2.78	17.57%
RF	0.97	1.30	0.90	5.09%	0.88	2.52	1.69	9.66%
XGB	0.99	0.06	0.01	0.05%	0.90	2.31	1.48	7.94%

The XGBoost model was utilized for SHAP analysis. In this study, each input parameter's importance was evaluated utilizing the mean SHAP value. Fig. 3. represents the mean absolute SHAP values for different features, ranking their overall impact on the ML model's predictions. The results show that Age has the highest impact with a SHAP value +18.24). The maximum positive value which indicates the major role CS. Similarly, Sand (+5.76), Cement (+5.37), and Silica Fume (+4.75) also exhibit a strong influence. The higher the mean SHAP value, the greater the feature's importance in determining the model's output. SHAP summary plot in Fig 3, showing both the magnitude and direction of feature influence on model predictions. Each point represents a single data instance, with colors indicating the feature values (red for high values, blue for low values). Features like Age, Silica Fume (SF), and Sand significantly impact the predicted mechanical properties, where higher values of Age and SF positively influence compressive strength.

Figure 4 illustrates the mean absolute SHAP values and provides a global explanation of the XGBoost model's predictions. Steel fiber exhibited the highest mean SHAP value (3.6), indicating its dominant influence on the Flexural Strength. Curing time (Age) followed with a SHAP value of 2.07, highlighting its significant impact. In contrast, Silica Fume had the least influence, with a SHAP value of 0.38. Additionally, SHAP analysis confirmed that the effect of cement was more substantial compared to sand and Superplasticizers (SP). Figure 4 illustrates that SHapley Additive exPlanations summary plot, which provides insights into the contribution of each input feature to the XGBoost model forecasts.

Steel fiber (SF), Age, and Coarse Aggregate (CA) have the most significant impact on the model output, with Steel fiber Age being the most influential feature. High values of Age and SF are indicate with positive SHAP values, and indicating a positive contribution to the FS prediction. Low values of SF and Age contribute negatively. The summary plot also includes combined contribution of less impactful features under "Sum of 8 other features" summarizing their combined effect on the model's prediction.

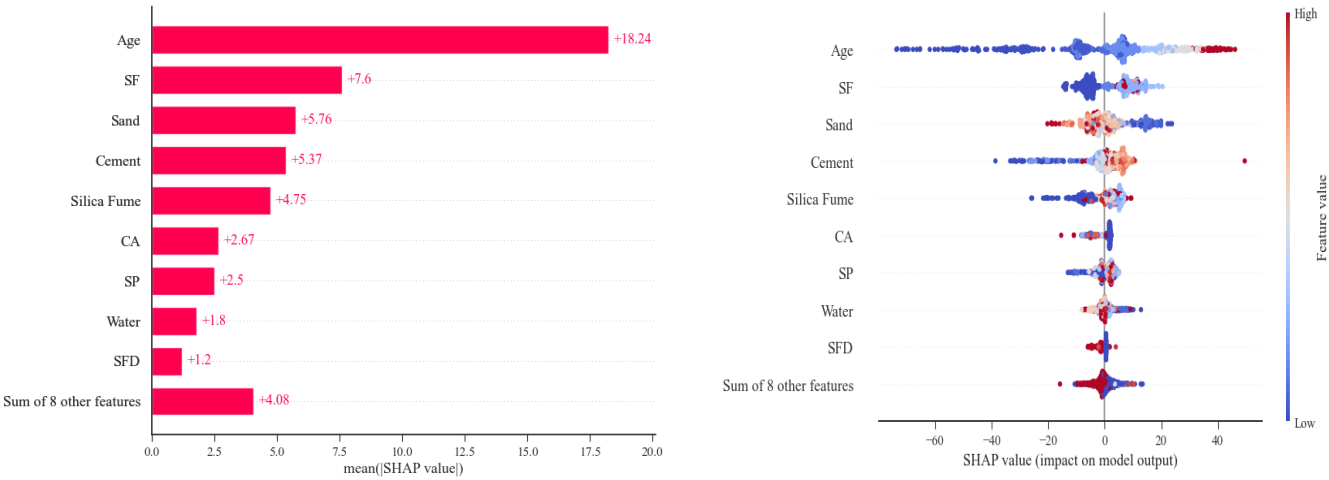

Figure 3. SHAP analysis of XGB model to predict FS: mean absolute SHAP values; and summary plot.

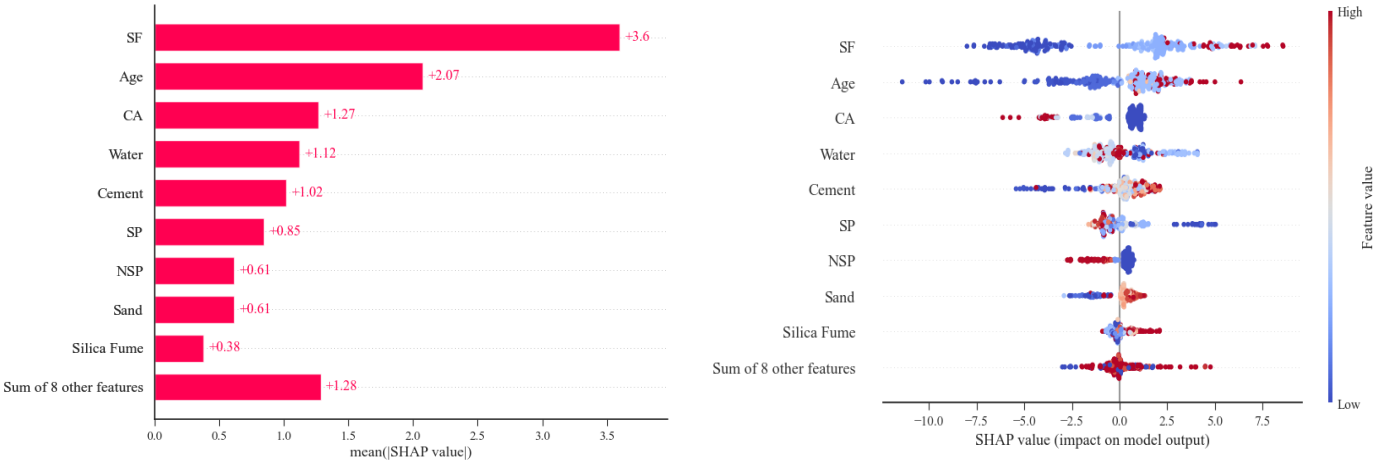

Figure 4. SHAP analysis of XGB model to predict FS: mean absolute SHAP values; and summary plot.

CONCLUSION

The present study comprehensively assessed the performance of advanced machine learning models (XGB, RF, and AdaBoost) in predicting the compressive strength (CS) and flexural strength (FS) of ultra-high-performance concrete (UHPC). A total of seventeen input parameters were selected to develop a robust predictive model for forecasting CS and FS. The dataset was randomly split into training set for 70% and remaining testing set for 30%, and model performance was evaluated using error metrics such as R^2, RMSE, MAE, and MAPE. The comparative analysis of ML models showed that XGBoost achieved the highest accuracy, with R^2 values of 0.93 for CS and 0.90 for FS, outperforming AdaBoost and RF. Additionally, XGBoost had the lowest error, with MAPE values of 5.79% for CS and 7.94% for FS. SHAP analysis of

the XGBoost model revealed that age, steel fiber, and cement were the most influential factors in predicting the compressive strength (CS) and flexural strength (FS) of UHPC. Artificial intelligence (AI) methods integrating on construction sites can help engineers accelerate processes and reduce dependence on traditional testing methods.

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