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Explainable machine learning based prediction of 28-day compressive strength of recycled aggregate self-compacting concrete using particle packing indicators.

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ABSTRACT
This study aims to develop an explainable machine learning framework for predicting the 28-day compressive strength of recycled aggregate self-compacting concrete (RA-SCC) using particle packing indicators. A dataset comprising 365 mixtures from 102 studies was analyzed using six regression models, with SHapley Additive exPlanations (SHAP) applied for interpretability. The Extra Trees model achieved the highest accuracy (R^2 = 0.9724, Root Mean Square Error (RMSE) = 1.19 MPa). The dataset is limited to 28-day strength and excludes admixture effects. The study introduces a combined approach integrating particle packing concepts, multicollinearity assessment, and explainable AI. The results demonstrate that machine learning can reliably predict strength while implicitly capturing packing-related mechanisms.
Keywords: recycled aggregate self-compacting concrete; machine learning; compressive strength prediction; particle packing indicators; explainable artificial intelligence; shap analysis; multicollinearity; sustainable concrete.

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Predicción explicable basada en aprendizaje automático de la resistencia a la compresión a 28 días de hormigón autocompactante de áridos reciclados utilizando indicadores de empaquetado de partículas.

RESUMEN

Este estudio tiene como objetivo desarrollar un marco entendible de aprendizaje automático para predecir la resistencia a compresión a 28 días del hormigón autocompactante de agregados reciclados (RA-SCC) utilizando indicadores de empaquetado de partículas. Se analizó un conjunto de datos que comprendía 365 mezclas de 102 estudios utilizando seis modelos de regresión, aplicando SHapley Additives ExPlanations (SHAP) para su interpretabilidad. El modelo Extra Trees alcanzó la mayor precisión (R2 = 0,9724, Root Mean Square Error (RMSE) = 1,19 MPa). El conjunto de datos está limitado a una resistencia a la compresión de 28 días y excluye efectos de mezclado. El estudio introduce un enfoque combinado que integra conceptos de empaquetado de partículas, evaluación de multicolinealidad e IA explicable. Los resultados demuestran que el aprendizaje automático puede predecir de forma fiable resistencia a la compresión mientras captura implícitamente los mecanismos relacionados con el empaquetado.

Palabras clave: concreto autocompactante de áridos reciclados; aprendizaje automático; predicción de resistencia a la compresión; indicadores de empaquetamiento de partículas; inteligencia artificial explicable; análisis de shap; multicolinealidad; hormigón sostenible.

Predição explicável, baseada em aprendizado de máquina, da resistência à compressão aos 28 dias do concreto autoadensável com agregados reciclados utilizando indicadores de empacotamento de partículas.

RESUMO

Este estudo tem como objetivo desenvolver uma estrutura de aprendizado de máquina explicável para prever a resistência à compressão aos 28 dias do concreto autoadensável com agregados reciclados (RA-SCC), utilizando indicadores de empacotamento de partículas. Um conjunto de dados composto por 365 misturas provenientes de 102 estudos foi analisado utilizando seis modelos de regressão, com aplicação do método SHapley Additive exPlanations (SHAP) para interpretação dos resultados. O modelo Extra Trees apresentou a maior precisão (R^2 = 0,9724; Raiz do Erro Quadrático Médio (RMSE) = 1,19 MPa). O conjunto de dados está limitado à resistência aos 28 dias e não considera os efeitos dos aditivos. O estudo apresenta uma abordagem combinada que integra conceitos de empacotamento de partículas, avaliação de multi-colinearidade e inteligência artificial explicável. Os resultados demonstram que o aprendizado de máquina pode prever a resistência de forma confiável, ao mesmo tempo em que captura implicitamente os mecanismos relacionados ao empacotamento de partículas.

Palavras-chave: concreto autocompactante de agregados reciclados; aprendizado de máquina; previsão de resistência à compressão; indicadores de empacotamento de partículas; inteligência artificial explicável; análise de shap; multicolinearidade; concreto sustentável.

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1. INTRODUCTION

Research on recycled aggregate concrete (RAC) as a potential substitute for regular concrete has increased due to the rising demand for environmentally friendly building materials. Utilizing recycled aggregates lessens the consumption of natural resources and lessens waste from construction and demolition, which is a major global environmental burden (Behera et al., 2014; Evangelista & de Brito, 2007; Silva et al., 2015). Due to its excellent flowability, passing ability, and resistance to segregation, self-compacting concrete (SCC) has become a cutting-edge building material that can be placed effectively in heavily reinforced structures without experiencing mechanical vibration (Khayat, 2016; Okamura & Ouchi, 2003). The integration of recycled aggregates into SCC offers substantial sustainability benefits; however, it also introduces pronounced variability in fresh and hardened properties, particularly compressive strength (Kou & Poon, 2009; Poon et al., 2004).

Compressive strength remains a primary design and quality control parameter in concrete engineering, directly influencing structural safety and serviceability. A complex interplay of material properties, such as the recycled aggregate replacement ratio, binder composition, water to binder ratio, aggregate grading, and additive dosage, controls the strength development of recycled aggregate self-compacting concrete (RA-SCC) (Guo et al., 2018; Tam et al., 2007; Xiao et al., 2012). The presence of adhered mortar on recycled aggregates alters particle morphology, water absorption, and interfacial transition zone behavior, thereby affecting particle packing efficiency and internal pore structure (Butler et al., 2013; Etxeberria et al., 2007). These coupled effects make reliable strength prediction using conventional empirical formulations particularly challenging.

Particle packing theory provides a mechanistic framework for understanding strength evolution in cementitious materials. Dense packing of solid constituents minimizes voids, enhances particle contact, and improves stress transfer within the hardened matrix (de Larrard, 1999; Funk & Dinger, 1994). Optimized aggregate packing can dramatically increase durability, compressive strength, and elastic modulus while lowering binder demand, according to experimental research (Cheng et al., 2021; He et al., 2022; Su et al., 2001). In SCC systems, packing density is especially critical because workability and segregation resistance are closely linked to volumetric balance among aggregates, fines, and paste (Felekoğlu et al., 2007; Khayat, 2016). Despite these advances, most particle packing approaches rely on labor intensive experimental procedures and are difficult to generalize across different material sources and mix designs.

Simultaneously, the use of machine learning (ML) techniques to simulate intricate and nonlinear interactions in concrete materials has grown in popularity (Tang et al., 2023). Artificial neural networks, support vector regression, random forest, and gradient boosting algorithms have all been successfully used in numerous studies to predict compressive strength more accurately than conventional regression models (Asteris et al., 2020; Liu et al., 2021; Yeh, 1998). The effectiveness of ensemble learning techniques for managing material variability and nonlinear interactions has been validated by recent studies concentrating on RAC (Li et al., 2022; Park et al., 2022). Nevertheless, a lot of machine learning models are viewed as "black boxes," which restricts their interpretability and undermines confidence in their use in engineering decision-making (Bardhan et al., 2021; Zhou et al., 2024).

Explainable artificial intelligence methods, including SHapley Additive exPlanations (SHAP), have been developed to quantify the impact of individual input variables to machine learning predictions to overcome this restriction (Lundberg & Lee, 2017). Concrete strength prediction has benefited from the effective use of SHAP-based interpretation, which provides physically meaningful insights into the role of mix constituents like cement, water content, and additional

cementitious ingredients (Almutairi, 2025; Fanijo et al., 2023). Although particle packing theory has been extensively investigated in concrete mix design, its integration with explainable machine learning approaches for recycled aggregate self-compacting concrete remains relatively limited.
Moreover, concrete mix design variables associated with particle packing are often strongly interdependent. Parameters such as aggregate fractions, fines content, and water to binder ratio exhibit significant multicollinearity, which undermines the reliability of linear statistical models and complicates physical interpretation (Kim & Lee, 2023; Li et al., 2022; J. Zhang et al., 2019). Even though multicollinearity has significant consequences for model selection and interpretability, it is rarely explicitly measured in ML-based concrete investigations. The research currently in publication, however, does not provide a comprehensive paradigm for RA-SCC strength prediction that concurrently addresses prediction accuracy, multicollinearity, and physical interpretability.
Considering this, the current study incorporates particle packing indicators derived from mix composition characteristics into a machine learning based framework for forecasting the compressive strength of RA-SCC. Unlike studies that explicitly calculate packing density or void ratio, this work captures packing related mechanisms implicitly through data driven modeling and interprets their influence using SHAP analysis. In addition, variance inflation factor analysis is employed to quantify multicollinearity among packing-related variables, providing a statistically robust basis for model selection. By integrating predictive accuracy, statistical validation, and physical interpretability, this study aims to contribute a reliable and explainable tool for sustainable RA-SCC mix design. It is recognized that particle packing behavior in concrete is governed by multiple interacting mix design variables, and may not be fully represented by individual packing indices alone. Several previous studies have investigated the effect of recycled aggregate replacement on compressive strength, establishing it as a key parameter in sustainable concrete design (Kou & Poon, 2009; Pedro et al., 2017; Xiao et al., 2012). These studies consistently highlight the influence of replacement level on strength reduction and variability, providing a basis for its inclusion as a primary input variable in predictive modeling frameworks.

2. RESEARCH OBJECTIVES.

This study's main goal is to create a machine learning framework that can accurately and interpretably forecast the compressive strength of RA-SCC by adding particle packing indicators that are obtained from characteristics related to mix composition. To achieve this aim, the following specific objectives are defined:

1. To compile and analyze a literature-based dataset of RA-SCC incorporating mix design variables associated with particle packing behavior, including aggregate proportions, binder content, water-to-binder ratio, volumetric indices, and recycled aggregate replacement level.
2. To create and evaluate many machine learning regression models for RA-SCC compressive strength prediction, such as ensemble, tree-based, and linear algorithms.
3. To evaluate model performance using comprehensive statistical indicators, including coefficient of determination, error based metrics, mean bias error, and hypothesis testing, to assess predictive accuracy and statistical reliability.
4. To use variance inflation factor analysis to measure the degree of multicollinearity among input variables linked to particle packing and investigate the implications for prediction stability and model selection.
5. To connect machine learning results with physically significant material behavior by

interpreting the impact of particle packing indicators on compressive strength prediction using SHapley Additive exPlanations.
6. To demonstrate the capability of explainable machine learning to implicitly capture particle packing mechanisms without explicit calculation of packing density or void ratio, supporting sustainable and data-driven RA-SCC mix design.

3. MATERIALS AND DATASET DESCRIPTION

3.1 Data source and compilation strategy.

The experimental results published in peer-reviewed literature on recycled aggregate concrete and recycled aggregate self-compacting concrete were systematically compiled to create the dataset used in this investigation. Only studies presenting complete and clearly defined mix proportions, material characteristics, and compressive strength values were considered. This approach ensured data reliability while capturing a wide range of material combinations and performance levels. The finalized dataset comprises N = 365 concrete mixtures, systematically compiled from 102 independent peer-reviewed research studies. Each selected study provided complete and consistent information on mix proportions and compressive strength, ensuring data quality and comparability across different experimental programs. The dataset spans a wide range of recycled aggregate replacement levels, binder compositions, and mixture configurations, thereby capturing realistic material variability. This diversity enhances the statistical representativeness and robustness of the machine learning framework developed in this study. The dataset is composed exclusively of experimentally measured compressive strength values reported in the source studies. No synthetic or simulated data were used. In addition to the training–testing split adopted in this study, the use of external experimental datasets for independent validation is recognized as an important step for future work to further assess model generalization across unseen material systems.

It is acknowledged that machine learning models developed using data from a single, well-controlled experimental program may provide higher internal consistency. However, the use of a literature-derived dataset in this study enables the incorporation of a broader range of material properties, mix proportions, and experimental conditions. This diversity enhances the generalizability of the developed model and allows it to capture realistic variability encountered in practical applications. Given the inherent complexity and interdependence of variables in recycled aggregate self-compacting concrete, the use of multiple independent data sources provides a more comprehensive representation of material behavior. The adopted approach is therefore intended to establish a generalized predictive framework rather than a project-specific model calibrated for a single experimental dataset. The selected studies span different recycled aggregate sources, replacement ratios, binder systems, and curing conditions, providing sufficient variability for robust machine learning analysis (Ajdukiewicz & Kliszczewicz, 2002; Limbachiya et al., 2000; Xiao et al., 2012).

The primary sources include experimental investigations on the mechanical behavior of recycled aggregate concrete, the influence of aggregate replacement level, and the role of supplementary cementitious materials such as fly ash. These studies collectively represent both conventional and high performance concrete systems and reflect realistic material variability encountered in practice (Corinaldesi, 2010; Kou & Poon, 2013; Pedro et al., 2017). Comprehensive reviews and monographs on recycled aggregate concrete were also used to ensure consistency in material definitions and experimental scope (de Brito & Saikia, 2013; Oikonomou, 2005). A detailed list of the references used for dataset compilation is provided in the References section. These sources collectively cover a wide range of recycled aggregate contents, binder systems, and testing conditions, ensuring that the dataset reflects realistic experimental variability reported in the literature.

3.2 Constituent materials.

3.2.1 Recycled aggregates.

Recycled aggregates used in the compiled studies were primarily obtained from crushed concrete waste originating from demolished structural elements. These aggregates typically consist of natural aggregate particles coated with adhered cement mortar, which alters surface texture, porosity, and water absorption characteristics compared to natural aggregates (Etxeberria et al., 2007; Poon et al., 2004). Several studies reported pre-treatment or beneficiation methods, such as mechanical processing or microwave-assisted techniques, to improve recycled aggregate quality; however, untreated aggregates were more commonly used to reflect practical construction scenarios (Akbarnezhad et al., 2011; Tam et al., 2005).
The recycled aggregate replacement ratio varied across studies, ranging from partial to full replacement of natural coarse aggregates. This variation is essential for evaluating the influence of recycled aggregate content on particle packing efficiency and compressive strength development (Evangelista & de Brito, 2007; Pedro et al., 2017). These effects are well documented in previous studies examining the influence of recycled aggregates on mechanical performance and microstructural characteristics of concrete (Butler et al., 2013; Etxeberria et al., 2007; Poon et al., 2004).

3.2.2 Cementitious materials.

Ordinary Portland cement (OPC) was the primary binding material employed in the experimental studies used for dataset compilation. In the compiled dataset, the term OPC refers to cementitious binders reported in the original studies, which may include both pure Portland cement (CEM I) and blended cements (such as CEM II) depending on the source. Due to variations in reporting practices across the literature, it was not always possible to explicitly distinguish between these cement types for all entries. OPC plays a fundamental role in governing the hydration process, paste formation, and early age strength development of RA-SCC. Variations in cement content directly influence paste volume, degree of particle coating, and load transfer capacity within the hardened matrix, all of which are closely linked to compressive strength performance.
Several studies incorporated supplementary cementitious materials, particularly fly ash, as partial replacement of cement. The inclusion of fly ash has been widely reported to enhance the long-term mechanical performance and durability of recycled aggregate concrete by refining pore structure and improving the interfacial transition zone between aggregate particles and cement paste (Behera et al., 2014; Kou & Poon, 2013). The spherical morphology and fine particle size of fly ash contribute to improved particle packing by filling micro voids between coarser particles, thereby increasing packing density and reducing capillary porosity.
From a particle packing perspective, cement and fly ash collectively control paste availability and fines distribution within the concrete system. Adequate paste volume is essential in self-compacting concrete to ensure proper flowability, segregation resistance, and complete encapsulation of aggregate particles. In RA-SCC, this requirement becomes more critical due to the higher surface roughness and water absorption associated with recycled aggregates. Fly ash contributes to improved workability and reduced water demand, indirectly influencing packing efficiency and internal void structure (de Brito & Saikia, 2013). These findings are consistent with established literature on the role of supplementary cementitious materials in enhancing durability and microstructural refinement in recycled aggregate concrete systems (Behera et al., 2014; Kou & Poon, 2013; Silva et al., 2015).
It should be noted that in several source studies, blended cement systems (e.g., CEM II) may

already contain supplementary cementitious materials such as fly ash. When such cements are reported alongside additional fly ash content, the effective contribution of fly ash may be overestimated. This introduces a degree of inherent bias in the dataset, leading to inflated apparent fly ash values and strong statistical interdependence among binder-related variables. This effect contributes directly to the extremely high VIF observed for fly ash content, reflecting severe multicollinearity among cementitious components. However, such interdependence is characteristic of literature-derived concrete datasets, where binder composition is governed by practical mix design constraints rather than independently controlled variables. The use of tree-based ensemble machine learning models in this study mitigates this limitation, as these algorithms are inherently robust to multicollinearity and do not rely on independent predictor assumptions.

In the compiled dataset, cement and fly ash contents exhibited strong interdependence with other mix design parameters, such as water to binder ratio and aggregate fractions. This interaction highlights their dominant role in defining the microstructural arrangement of solid particles and hydration products. Consequently, cement and fly ash contents were treated as key particle packing indicators in the machine learning framework, enabling the models to implicitly capture packing-related mechanisms affecting compressive strength development.

3.2.3 Aggregates and mixing water.

Both coarse and fine aggregates were included in the dataset, with fine aggregate typically consisting of natural river sand. Aggregate grading and volumetric proportions were reported explicitly in most studies, enabling the derivation of aggregate fractions and aggregate volume fraction parameters (Domingo-Cabo et al., 2009; Limbachiya et al., 2000). Mixing water content and water-to-binder ratio were extracted directly, as these parameters strongly affect workability, void structure, and compressive strength (Poon et al., 2004; Tam et al., 2005). In self-compacting concrete, chemical admixtures such as superplasticizers and viscosity modifying agents play a crucial role in achieving the required flowability, passing ability, and resistance to segregation. However, these parameters were not consistently reported across the compiled literature sources and were therefore not included as input variables in the present machine learning framework. This omission represents a limitation, as admixture dosage significantly influences both fresh and hardened properties of SCC.

In self-compacting concrete systems, fresh state properties such as flowability, passing ability, and resistance to segregation are essential performance criteria. These characteristics are typically evaluated using standardized tests including slump flow, V-funnel, and L-box tests. Variations in mix composition, particularly aggregate proportions, binder content, and water-to-binder ratio, significantly influence these properties. However, due to the lack of consistently reported fresh property data in the compiled literature sources, the present study focuses exclusively on compressive strength prediction. In addition, key parameters distinguishing self-compacting concrete from conventional concrete such as high range water reducing admixture dosage, viscosity modifying agent content, and void related rheological characteristics were not consistently available in the compiled dataset. Consequently, the model does not explicitly differentiate SCC behavior based on fresh state performance but rather captures its effects indirectly through mix composition variables.

3.3 Input and output variables.

A set of input variables representing material composition and particle packing properties was created based on the published experimental results. The dataset used for model development consists of 365 samples, providing a sufficiently large and diverse basis for reliable machine learning training and validation. These include cement content, fly ash content, coarse aggregate content, fine aggregate ratio, recycled aggregate replacement percentage, water content, water to binder ratio, aggregate volume fraction, packing index, and curing age. Although particle packing density or void ratio was not explicitly calculated in the source studies, these variables collectively act as particle packing indicators, as they govern the spatial distribution of solid particles and paste within the concrete matrix (Cheng et al., 2021; de Brito & Saikia, 2013).

The concrete's compressive strength, as determined at predetermined curing ages and under controlled laboratory settings, is the output variable. Compressive strength values were reported consistently across the selected studies, allowing meaningful comparison and aggregation (Ajdukiewicz & Kliszczewicz, 2002; Corinaldesi, 2010). Compressive strength was taken into consideration as the output parameter, and a set of factors relating to material composition and particle packing were chosen as model inputs based on the collected literature dataset. The complete list of input and output variables, including their symbols, units, and functional roles in the machine learning framework, is summarized in Table 1. Basic descriptive statistics were calculated for the collected dataset in order to shed light on the distribution and variability of the input and output variables needed for machine learning modeling. The minimum, maximum, mean, standard deviation, and variance of each variable are summarized in Table 2.

Table 1. Description of input and output variables used for machine learning modeling.

Variable	**Symbol**	**Unit**	**Description**	**Role in model**
Age	Age	Days	Concrete specimens' curing period	Input
Cement	Cement	kg/m³	Ordinary Portland cement content in the mixture	Input
Fly ash	FA	kg/m³	Content of fly ash used as supplementary cementitious material	Input
Coarse aggregate	CA	kg/m³	The concrete mixture's coarse aggregate content	Input
Water	Water	kg/m³	Mixing water content	Input
Water-to-binder ratio	W/B	–	Ratio of total mixing water to total binder content	Input
Recycled aggregate content	RA (%)	%	Percentage replacement of natural aggregate by recycled aggregate	Input
Fine aggregate ratio	FAR	–	The proportion of total aggregate content to fine aggregate	Input
Aggregate volume fraction	AVF	–	Aggregates' volume percentage in the concrete mixture	Input
Packing index	PI	–	Index representing particle packing efficiency	Input
Compressive strength	CS	MPa	Concrete's measured compressive strength	Output
Water	Water	kg/m³	Mixing water content	Input
Water-to-binder ratio	W/B	–	Ratio of total mixing water to total binder content	Input

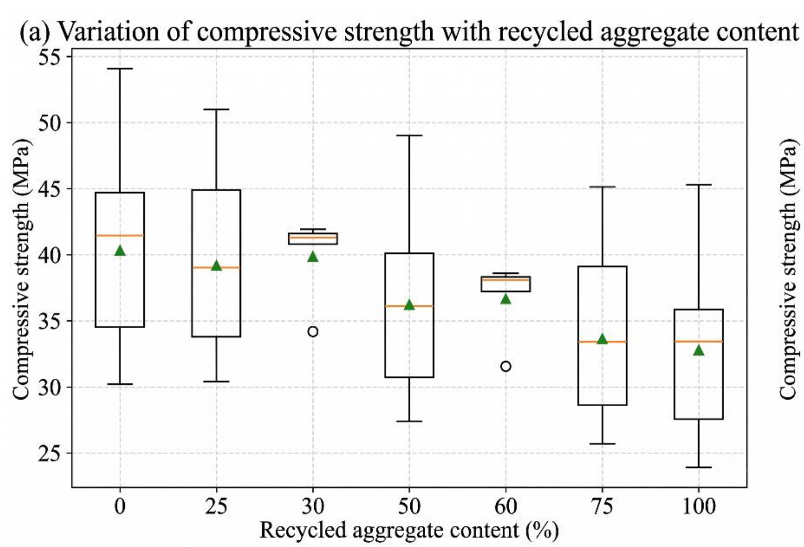
Note: *FAR denotes fine aggregate ratio, AVF denotes aggregate volume fraction, PI denotes packing index, and W/B denotes water-to-binder ratio.*

Table 2. Statistical summary of dataset variables used in the study.

Input parameter	Min	Max	Mean	Std. dev.	Variance
Age (days)	28	28	28	0	0
Cement (kg/m³)	300	511.9	352.249	33.001	1089.069
Fly ash (kg/m³)	511	780	716.027	41.548	1726.209
Coarse aggregate (kg/m³)	980	1330	1069.904	46.106	2125.783
Water (kg/m³)	155.1	215	171.202	6.618	43.796
Water-to-binder ratio (W/B)	0.38	0.58	0.491	0.052	0.003
Recycled aggregate content (%)	0	100	48.932	39.757	1580.586
Fine aggregate ratio (FAR)	0.31	0.407	0.401	0.011	0
Aggregate volume fraction (AVF)	0.613	0.728	0.663	0.019	0
Packing index (PI)	7.67	12.61	10.475	0.515	0.265
Compressive strength (MPa)	23.9	54.1	36.591	6.79	46.102

Note: *Std. dev. denotes standard deviation. All compressive strength values correspond to a curing age of 28 days. It is important to note that the dataset used in this study is restricted to a single curing age of 28 days, resulting in no variability in the age parameter. Consequently, the developed machine learning models are specifically designed to predict the 28-day compressive strength of recycled aggregate self-compacting concrete, rather than capturing strength evolution over time. FAR denotes fine aggregate ratio, AVF denotes aggregate volume fraction, PI denotes packing index, and W/B denotes water-to-binder ratio.*

While 28-day compressive strength is widely accepted as the standard reference for structural design and quality control in concrete engineering, this limitation implies that the proposed model does not explicitly account for time-dependent hydration processes. Supplementary cementitious materials such as fly ash are known to contribute to strength development beyond 28 days, often achieving significant strength gain at later curing ages such as 56 or 90 days. Therefore, the present study focuses on modeling the compressive strength at the standard 28-day curing period, which remains the most reported and practically relevant parameter in literature-based datasets. Future research should incorporate multi-age datasets to enable time-dependent modeling and to better capture the long-term hydration kinetics of blended cementitious systems.



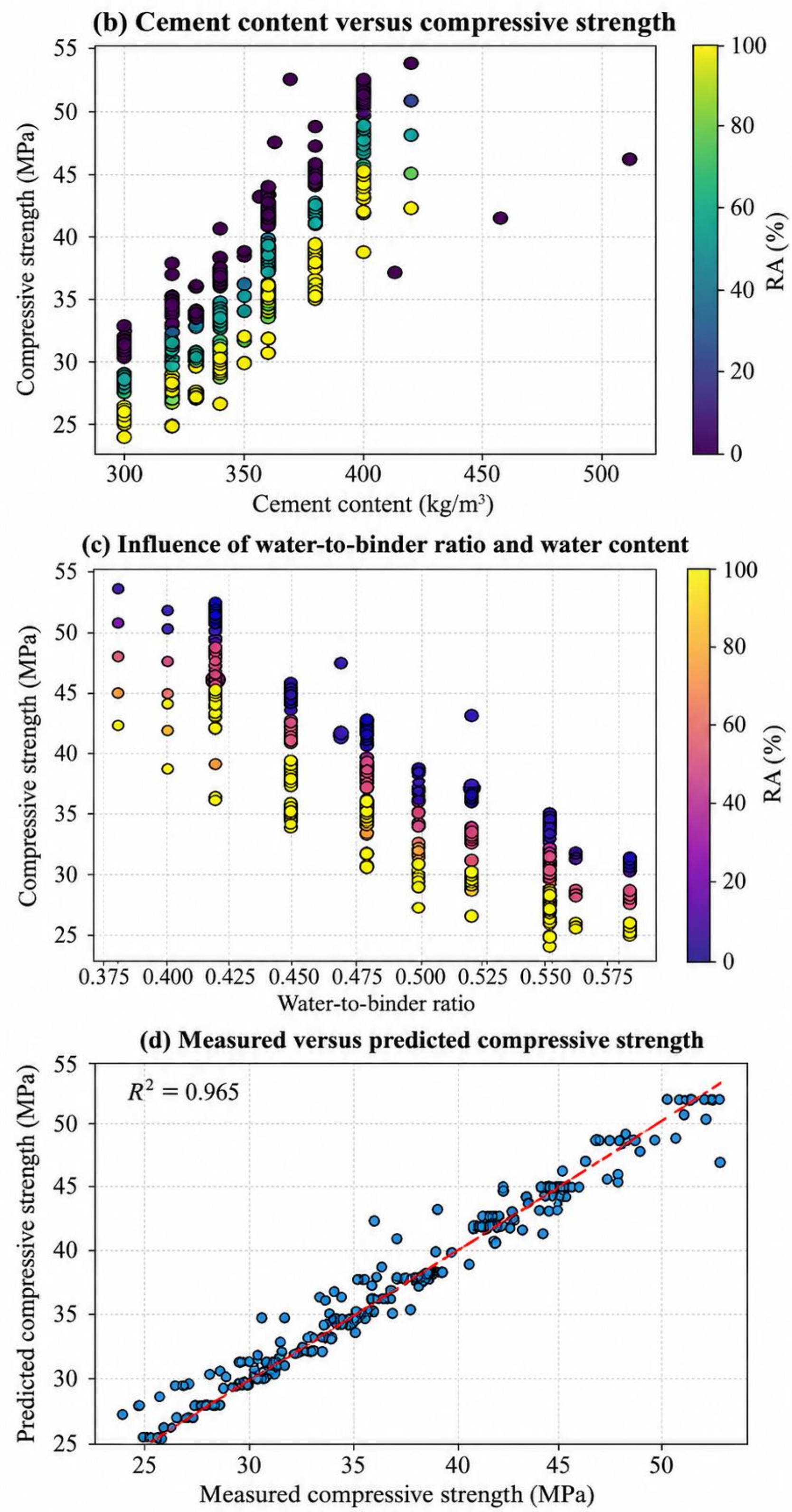


Figure 1. Dataset characterization illustrating (a) compressive strength variability with recycled aggregate content, (b) dependence of compressive strength on cement content under varying recycled aggregate levels, (c) combined effects of water to binder ratio and water content on compressive strength, and (d) measured versus predicted compressive strength based on combined input parameters ($R^2 = 0.965$).

Figure 1 presents a concise visual assessment of the recycled aggregate self-compacting concrete dataset prior to machine learning modeling. The effects of recycled aggregate content, cement dosage, and water-related parameters on compressive strength are illustrated in Fig. 1(a-c), highlighting material variability and coupled mix design influences. With a high coefficient of determination, Figure 1(d) demonstrates a remarkable correlation between the observed and anticipated compressive strength using the combined input parameters (R^2 = 0.965), confirming that the dataset effectively captures the key mechanisms governing strength development.

3.4 Data preprocessing and consistency.
To ensure compatibility across different experimental programs, all input variables were converted to consistent units and normalized prior to machine learning analysis. Data entries with incomplete mix information or ambiguous testing conditions were excluded. The machine learning models may learn both individual impacts and interacting behaviors related to particle packing because the final dataset shows a balanced distribution of recycled aggregate contents, binder compositions, and water to binder ratios.
This literature-based dataset maintains a close connection to the behavior of recycled aggregate concrete systems as observed in experiments, while offering a physically meaningful basis for data-driven modeling.

4. METHODOLOGY

The workflow of the suggested machine learning framework created to forecast the compressive strength of RA-SCC concrete is shown in Figure 2. The process begins with the compilation of a literature-based dataset and proceeds through data preprocessing, normalization, and dataset partitioning. Multicollinearity among particle packing related variables is quantified using variance inflation factor analysis prior to model development. After that, statistical performance metrics and hypothesis testing are used to train and assess multiple regression and ensemble machine learning models. Finally, SHapley Additive exPlanations are employed to interpret model predictions and identify the most influential particle packing indicators, ensuring both predictive accuracy and physical interpretability.

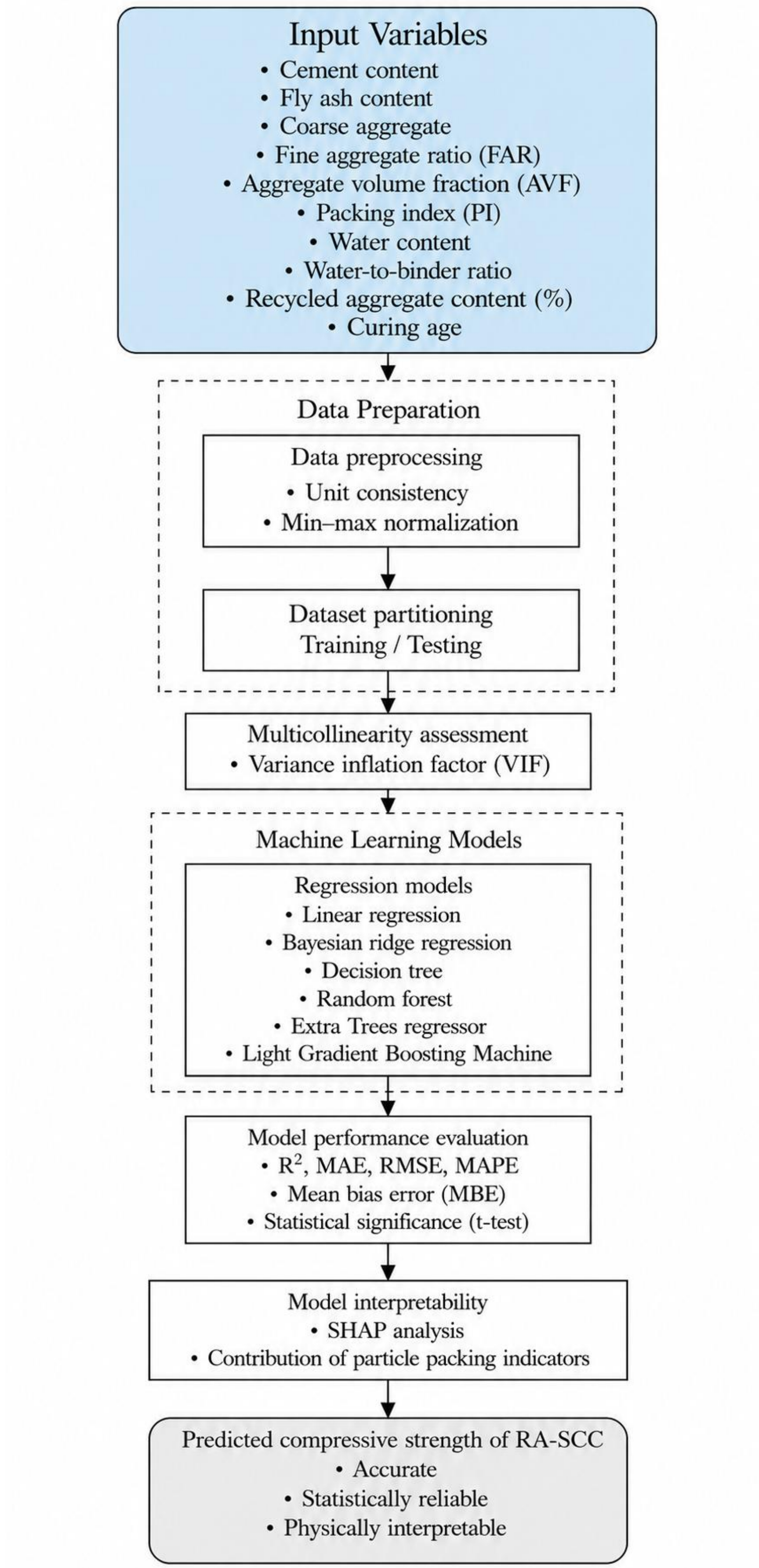


Figure 2. Workflow of the proposed machine learning framework.

4.1 Overview of the proposed methodology.

Strong nonlinearity, multicollinearity, and material variability are inherent in RA-SCC, and the scientific approach used in this study was created to comprehensively address these difficulties. The methodology was divided into four consecutive and connected steps: data preprocessing and normalization, multicollinearity assessment, machine learning model development, and performance evaluation with explainable analysis. This was done to guarantee both predictive accuracy and engineering interpretability.

In the first stage, the compiled literature-based dataset was subjected to preprocessing to ensure consistency, numerical stability, and compatibility across different experimental sources. This step is critical in data-driven modeling of concrete properties, as raw experimental data often exhibit wide variations in scale and distribution that can adversely affect model learning and convergence (Liu et al., 2021; Yeh, 1998). Normalization of input variables also facilitates fair comparison among different machine learning algorithms.

Using variance inflation factor (VIF) analysis, the second stage concentrated on quantifying the interdependencies among input variables. Mix design parameters associated with particle packing, such as aggregate fractions, binder content, and water to binder ratio, are often highly correlated. Explicit evaluation of multicollinearity provides a statistical basis for understanding the limitations of linear regression models and supports the selection of nonparametric and ensemble learning approaches that are more robust to correlated inputs (Kutner et al., 2005; Li et al., 2022).

To capture the intricate and nonlinear interactions between particle packing indicators and compressive strength, many machine learning regression models were created in the third step. Both traditional regression methods and sophisticated tree-based ensemble models were used to allow for comparison and to investigate how algorithmic complexity affected prediction results (Asteris et al., 2020).

The final stage integrated comprehensive performance evaluation with explainable artificial intelligence techniques. In addition to conventional accuracy and error metrics, statistical bias assessment and hypothesis testing were employed to evaluate model reliability. Furthermore, SHapley Additive exPlanations (SHAP) were used to interpret model predictions and quantify the contribution of individual particle packing indicators, thereby linking data-driven results with physically meaningful material behavior (Almutairi, 2025; Lundberg & Lee, 2017). This integrated methodology ensures that the developed framework is not only accurate but also transparent and suitable for engineering application.

4.2 Data normalization and dataset partitioning.

All input features were normalized using min-max scaling to increase numerical stability during model training and lessen the impact of scale discrepancies across input variables. The normalization procedure is expressed as:

$$x_{\text{norm}} = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \quad (1)$$

where x denotes the original value of an input feature, and $x_{\min}$ and $x_{\max}$ indicate the feature's lowest and maximum values in the dataset. Feature normalization is particularly important for regression algorithms that involve distance calculations or iterative optimization, as it prevents variables with larger numerical ranges from dominating the learning process (Liu et al., 2021; Yeh, 1998).

Following normalization, the dataset was randomly partitioned into training and testing subsets to evaluate the generalization capability of the developed machine learning models. 30% of the dataset in this study was put aside for independent testing, while the remaining 70% was used for model training and hyperparameter tweaking. The training subset was used exclusively for model calibration and hyperparameter tuning, whereas the testing subset was not involved in any stage of model development. This strategy minimizes information leakage and enables a rigorous assessment of predictive performance on unseen data, which is particularly important for literature-based datasets characterized by material variability.

4.3 Multicollinearity assessment using variance inflation factor.

Concrete mix parameters associated with particle packing are often strongly correlated, which can adversely affect model stability and interpretability. To quantify the degree of multicollinearity among input variables, the VIF was computed for each feature. VIF is defined as:

$$\mathrm{VIF}_i = \frac{1}{1-R_i^2} \tag{2}$$

where R_i^2 is the coefficient of determination obtained by regressing the i^{th} predictor against all remaining predictors. A VIF value greater than 10 generally indicates severe multicollinearity (Kutner et al., 2005; Li et al., 2022). To quantify the degree of multicollinearity among the particle packing related input variables, VIF values were computed. The resulting VIF values for each predictor variable are presented in Table 3. Such extreme VIF values indicate that conventional coefficient based interpretation is unreliable, thereby reinforcing the suitability of tree based ensemble models for this problem.

Table 3. Variance inflation factor (VIF) values of input variables.

Input variable	VIF value
Cement	137.495
Fly ash (FA)	1405.819
Coarse aggregate (CA)	580.775
Water-to-binder ratio (W/B)	240.825
Water	19.978
Recycled aggregate content (RA %)	1.025
Fine aggregate ratio (FAR)	777.145
Aggregate volume fraction (AVF)	35.664
Packing index (PI)	12.89

Note: *VIF values greater than 10 indicate severe multicollinearity among predictor variables. FAR denotes fine aggregate ratio, AVF denotes aggregate volume fraction, PI denotes packing index, and W/B denotes water-to-binder ratio.*

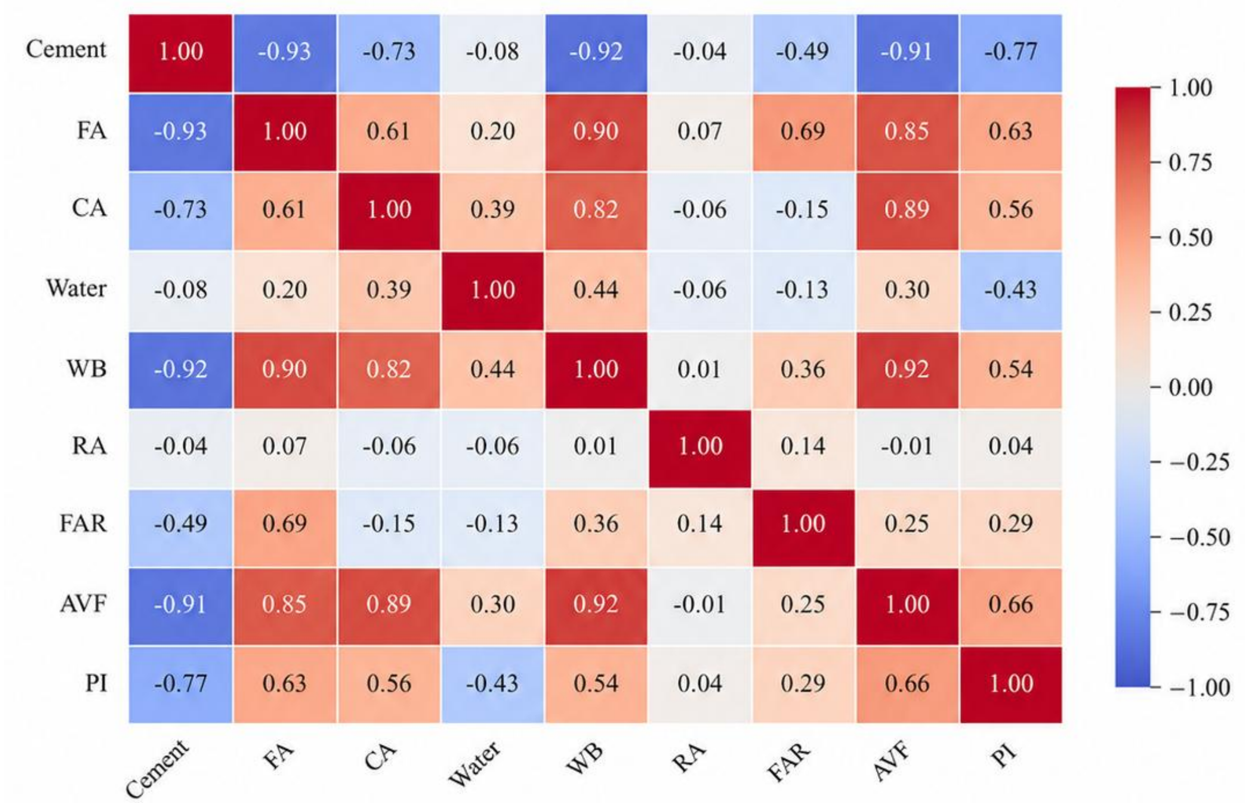


Figure 3. Correlation matrix of particle packing related input variables used for compressive strength prediction of compressive strength of RA-SCC.

The Pearson correlation matrix for the input factors related to particle packing that were taken into consideration in this investigation is shown in Figure 3. The presence of multicollinearity is indicated by the strong correlations found between a number of binder and aggregate related variables. This is quantitatively investigated using variance inflation factor analysis in the following section to evaluate its implications for model stability and selection. Significant interdependence between binder composition, paste quality, and volumetric packing characteristics is indicated by the strong negative correlations found between cement content and fly ash content ($r = -0.93$), water to binder ratio ($r = -0.92$), and aggregate volume percent ($r = -0.91$). The fly ash concentration, on the other hand, shows substantial positive relationships with the aggregate volume fraction ($r = 0.85$) and water to binder ratio ($r = 0.90$), indicating the combined involvement of paste dispersion and fines content in self-compaction concrete mixtures.

The volumetric restrictions controlling particle packing are highlighted by the moderate to significant correlations observed between coarse aggregate content and the water to binder ratio ($r = 0.82$) and aggregate volume fraction ($r = 0.89$). Recycled aggregate content's relative statistical independence within the dataset is confirmed by its minor correlations with every other variable. Significant multicollinearity is indicated by the strong inter-variable correlations between binder- and aggregate-related parameters. This supports the use of tree-based and ensemble machine learning models for robust strength prediction and justifies the subsequent variance inflation factor analysis.

4.4 Machine learning regression models.

To forecast the compressive strength of recycled aggregate self-compaction concrete, six regression models were created.

4.4.1 Linear regression and bayesian Ridge Regression.

According to the linear regression model, input factors and compressive strength have a linear relationship, which is represented as follows:

$$\hat{y} = \beta_0 + \sum_{i=1}^{n} \beta_i \, x_i \tag{3}$$

where $\hat{y}$ is the predicted compressive strength, x_i represents the input variables, and β_i are regression coefficients.

Bayesian ridge regression extends this formulation by introducing probabilistic priors on the regression coefficients to improve numerical stability under multicollinearity (Montgomery et al., 2012).

4.4.2 Decision tree based models.

Recursively dividing the input feature space into a collection of disjoint sections is how decision tree regression, a nonparametric supervised learning method, models nonlinear connections. At each internal node of the tree, the dataset is split based on a selected input variable and a corresponding threshold value, with the objective of minimizing prediction error within the resulting subsets. Until predetermined ending requirements, like the minimum number of samples per node or the maximum tree depth, are met, this recursive binary splitting procedure keeps going.

The mean of the observed values corresponding to the samples lying within a specific terminal node (leaf) is used to calculate the anticipated compressive strength for that node. A decision tree model's prediction function can be written as follows:

$$\hat{y}(x) = \sum_{m=1}^{M} c_m \; \mathbb{I}(x \in R_m) \tag{4}$$

where M is the total number of terminal regions, R_m denotes the m^{th} region of the feature space, c_m represents the average compressive strength of samples within region R_m, and $\mathbb{I}(\cdot)$ is an indicator function that equals 1 when the condition is satisfied and 0 otherwise (Breiman et al., 1984).

In regression problems, the optimal split at each node is commonly determined by minimizing the variance or mean squared error of the target variable within the child nodes. Decision trees can capture intricate relationships between input variables thanks to this criterion, which eliminates the need for presumptions about their functional structure. Because particle packing indicators and mix design parameters interact in a highly nonlinear way in heterogeneous material systems like recycled aggregate self-compacting concrete, decision tree models are therefore ideally suited for modeling these systems (Asteris et al., 2020; Yeh, 1998).

4.4.3 Random forest and extra trees regressors.

An ensemble of decision trees trained on bootstrapped samples is created using random forest regression, and the final predictions are derived by averaging the outputs of each individual tree (Breiman, 2001):

$$\hat{y} = \frac{1}{M} \sum_{m=1}^{M} \hat{y}_m \tag{5}$$

where M is the number of trees and $\hat{y}_m$ is the prediction from the m^{th} tree.
The Extra Trees Regressor further increases randomness by selecting split thresholds randomly, which enhances generalization and reduces variance, particularly in datasets with correlated predictors.

4.4.4 Light gradient boosting machine.
A gradient boosting framework called Light Gradient Boosting Machine (LightGBM) constructs additive regression trees in a sequential fashion. The anticipated result is provided by:

$$\hat{y}_k = \sum_{t=1}^{T} f_t\,(x_k) \tag{6}$$

where f_t represents the t^{th} decision tree and T is the total number of boosting iterations (Ke et al., 2017). LightGBM is a computationally efficient tool that works well for simulating intricate relationships between particle packing indicators.

4.5 Model performance evaluation metrics.
To ensure a comprehensive and statistically reliable evaluation of model performance, multiple quantitative indicators were employed to assess prediction accuracy, error magnitude, systematic bias, and statistical consistency between predicted and experimental compressive strength values. The use of multiple evaluation metrics is essential in concrete strength prediction, as reliance on a single indicator may lead to misleading conclusions regarding model robustness (Montgomery et al., 2012; Willmott & Matsuura, 2005).
The coefficient of determination (R^2) was used to quantify the proportion of variance in the measured compressive strength explained by the model predictions. It is defined as:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2} \tag{7}$$

where y_i and $\hat{y}_i$ denote the experimentally measured and predicted compressive strength values for the i^{th} sample, respectively, $\bar{y}$ represents the mean of the measured values, and N is the total number of observations. A higher R^2 value indicates stronger agreement between predictions and experimental results.
The mean absolute error (MAE) was computed to assess absolute prediction error:

$$\text{MAE} = \frac{1}{N}\sum_{i=1}^{N} \mid y_i - \hat{y}_i \mid \tag{8}$$

MAE provides a direct measure of the average magnitude of prediction errors and is less sensitive to extreme values compared to squared error metrics. The root mean square error (RMSE), on the other hand, penalizes larger errors more severely and is represented as:

$$\text{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2} \tag{9}$$

In engineering applications, where greater deviations from measured values may have important structural ramifications, RMSE is especially helpful for evaluating model performance (Willmott & Matsuura, 2005).

To quantify systematic over or under prediction, the mean bias error (MBE) was computed as:

$$\text{MBE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i) \quad (10)$$

A tendency for underestimating is indicated by a positive MBE, whereas overestimation is shown by a negative value. Unbiased predictions, which are necessary for trustworthy engineering decision-making, are indicated by values near zero.
To determine whether the variations between the experimental and anticipated compressive strength values were statistically significant, a statistical hypothesis test was performed in addition to error-based metrics. The null hypothesis, according to which the mean difference between the measured and anticipated values is zero, was tested using a paired t-test. Statistical agreement was assessed using the resulting t-statistic and associated p-value; at the 95% confidence level, p-values larger than 0.05 indicated no significant difference (Montgomery et al., 2012). Confidence in the prediction reliability of the created machine learning models is increased by this statistical validation.

4.6 SHAP-based model interpretability.

SHapley Additive exPlanations (SHAP) were used to interpret the role of particle packing indicators in model predictions. SHAP values satisfy additivity and are derived from cooperative game theory:

$$f(x) = \phi_0 + \sum_{i=1}^{n}\phi_i \quad (11)$$

where ϕ_i represents the contribution of the i^{th} feature to the prediction (Lundberg & Lee, 2017). This approach enables quantification of both magnitude and direction of feature influence, allowing direct linkage between machine learning outputs and physical particle packing mechanisms. It is important to note that SHAP values quantify the contribution of input variables to model predictions rather than establishing strict physical causality. In datasets characterized by strong multicollinearity, such as the present study, correlated variables may share or redistribute their contributions across one another. As a result, the importance assigned to individual features should be interpreted with caution, particularly when high variance inflation factor (VIF) values are observed. In the current dataset, cement content, fly ash content, and water-to-binder ratio exhibit strong interdependence, reflecting practical constraints in concrete mix design rather than independent physical variables. Under such conditions, SHAP-based importance should be interpreted as a representation of the collective influence of correlated variables rather than isolated causal effects. Despite this limitation, the SHAP results obtained in this study remain physically meaningful, as the identified dominant variables recycled aggregate content, cement content, and water to binder ratio are well-established governing factors influencing compressive strength and particle packing behavior. The consistency between SHAP derived rankings and established concrete mechanics provides confidence that the model captures realistic material behavior, even in the presence of multicollinearity. Therefore, SHAP analysis in this study is interpreted as an explainability tool that provides insight into variable influence within a correlated system, rather than a strict causal attribution method. This distinction is essential for ensuring a scientifically rigorous interpretation of the results.

4.7 Computational implementation.

To guarantee reproducibility, transparency, and computational efficiency, Python-based scientific computing libraries were used for all data processing, machine learning modeling, and statistical analyses. Python was selected due to its extensive ecosystem of open source tools widely adopted in data-driven materials research and civil engineering applications (McKinney, 2010; Pedregosa et al., 2011).

The computational workflow comprised sequential stages, including data normalization, dataset partitioning, variance inflation factor computation, model development, performance evaluation, and explainable machine learning analysis. To provide fair performance comparison, feature normalization and preprocessing procedures were implemented uniformly across all models. Standardized library functions were used to develop machine learning algorithms, allowing for dependable and repeatable model training and testing processes.

Hyperparameter tuning was conducted within the training dataset using cross-validation to improve model generalization and to prevent overfitting. To prevent knowledge leaking and guarantee an objective evaluation of predicted performance, all trained models were only tested on the independent testing dataset. Statistical evaluation metrics and hypothesis testing were computed using established numerical libraries to maintain accuracy and numerical stability (Montgomery et al., 2012).

Model interpretability was achieved using SHapley Additive exPlanations, which were computed using efficient approximation algorithms compatible with tree-based models. This approach enables consistent attribution of feature contributions across individual predictions and global model behavior, facilitating meaningful interpretation of particle packing indicators influencing compressive strength (Lundberg & Lee, 2017). Intermediate stages of the modeling workflow, including data preprocessing, multicollinearity assessment, model training, and performance evaluation, were systematically validated using the training testing split approach. Cross-validation was employed during hyperparameter tuning to ensure model stability and to prevent overfitting. The reported results therefore reflect both model accuracy and generalization capability based on unseen testing data.

The use of open source software and standardized implementation practices ensures that the developed framework can be readily reproduced and extended by other researchers. This openness facilitates the future development of explainable machine learning models for sustainable concrete materials as well as their validation and benchmarking.

5. RESULTS AND DISCUSSION

5.1 Comparison of machine learning model performance.

Several statistical measures, such as coefficient of determination (R2), mean absolute error (MAE), root mean square error (RMSE), mean absolute percentage error (MAPE), mean bias error (MBE), and hypothesis testing, were used to assess the predictive performance of the six machine learning models. The findings unequivocally show that when it comes to forecasting the compressive strength of RA-SCC, ensemble-based models perform better than linear and single tree approaches.

With an R^2 value of 0.9724, the Extra Trees Regressor had the highest predictive accuracy of any model, meaning that it was able to account for over 97% of the variation in compressive strength. This model also exhibited the lowest MAE (0.79 MPa) and RMSE (1.19 MPa), demonstrating superior error minimization. With R^2 values of 0.968 and 0.965, respectively, the Random Forest and Light Gradient Boosting Machine models likewise demonstrated excellent performance. These results support earlier research on recycled aggregate concrete's conclusions that ensemble learning techniques are appropriate for simulating highly nonlinear concrete behavior (Ahmed et al., 2024; Asteris et al., 2020; Liu et al., 2021). Table 4 provides a summary of each model's coefficient of determination, error-based metrics, mean bias error, and hypothesis testing outcomes.

Table 4. Performance comparison of machine learning models for compressive strength prediction.

Model	R^2	MAE (MPa)	MSE (MPa^2)	RMSE (MPa)	MAPE (%)	MBE (MPa)	t-statistic	p-value
Linear regression	0.9526	1.336	2.444	1.563	3.8	-0.042	-0.282	0.779
Bayesian ridge regression	0.9146	1.525	4.404	2.099	4.13	-0.042	-0.211	0.833
Decision tree regressor	0.9363	1.167	3.28	1.811	3.06	0.203	1.177	0.242
Random forest regressor	0.968	0.855	1.648	1.284	2.31	0.095	0.771	0.443
Extra Trees regressor	0.9724	0.788	1.423	1.193	2.12	0.122	1.074	0.285
Light gradient boosting machine	0.965	0.866	1.802	1.343	2.3	0.205	1.61	0.11

Note: *MAE denotes mean absolute error, MSE denotes mean squared error, RMSE denotes root mean square error, MAPE denotes mean absolute percentage error, and MBE denotes mean bias error.*

The prediction accuracy and error levels of Bayesian Ridge Regression and Linear Regression were significantly lower. The main cause of this decline in performance is the mix design variables' significant interdependence, which goes against the presumptions of linear modeling. Previous studies on machine learning-based concrete strength prediction have documented similar limits of linear regression in the presence of multicollinearity (Li et al., 2022).
Scatter graphs comparing the experimental and projected compressive strength values for each of the six machine learning models taken into consideration in this investigation are shown in Figure 4. Tight data point clustering around the 45° reference line is a sign of good prediction accuracy and low bias in the ensemble-based models, especially the Extra Trees and Random Forest regressors. Strong agreement is also shown by the Light Gradient Boosting Machine, which exhibits somewhat greater dispersion at higher strength values. In contrast, linear regression, Bayesian ridge, and decision tree models show greater scatter, reflecting their reduced capability to capture nonlinear interactions among particle packing related variables. The visual patterns support the higher predictive reliability of ensemble learning techniques for recycled aggregate self-compaction concrete and are in line with the quantitative performance indicators listed in Table 4.

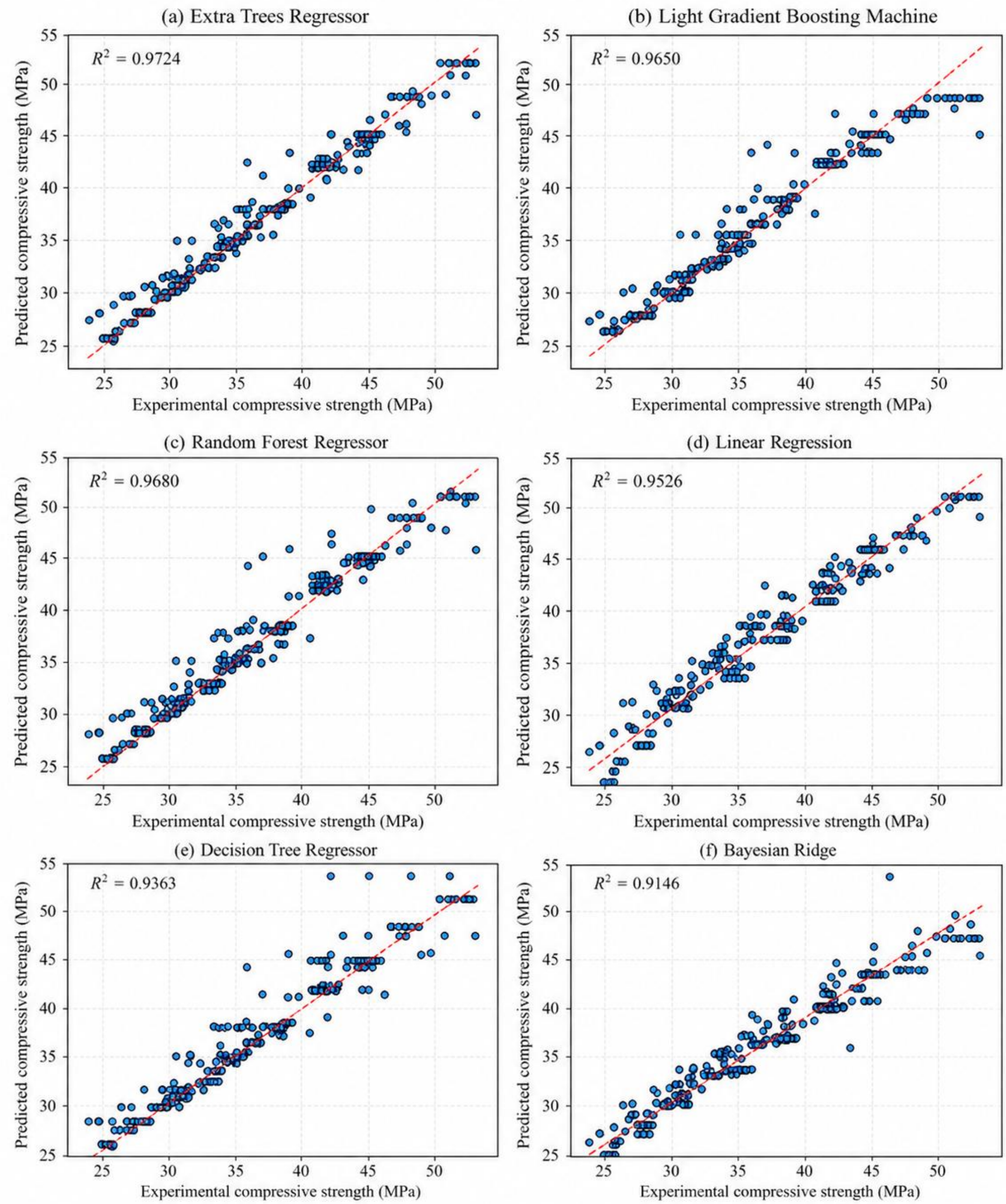


Figure 4. Comparison between predicted and experimental compressive strength obtained using different machine learning models: (a) Extra Trees regressor, (b) Light Gradient Boosting Machine, (c) random forest regressor, (d) linear regression, (e) decision tree regressor, and (f) Bayesian ridge regression.

Figure 5 presents the residual distributions obtained for all six machine learning models, providing insight into prediction bias and error dispersion beyond conventional accuracy metrics. The Extra Trees Regressor's low mean bias error (MBE = 0.122 MPa), tiny RMSE (1.19 MPa), and strong coefficient of determination (R2 = 0.9724) are all consistent with its narrowly dispersed, nearly symmetric residual profile that is centered at zero. Strong predictive stability is further confirmed by the Random Forest Regressor, which displays a compact residual spread with little bias (MBE = 0.0945 MPa; RMSE = 1.28 MPa). Although it exhibits slightly more dispersion, as evidenced by its higher RMSE of 1.34 MPa, the Light Gradient Boosting Machine similarly shows residuals centered near zero (MBE = 0.2046 MPa). In contrast, the linear regression and Bayesian ridge models display broader residual distributions despite near-zero bias values (MBE ≈ −0.04 MPa), indicating increased random error and reduced capability to represent nonlinear interactions among particle packing related variables. The decision tree regressor shows moderate asymmetry and dispersion, consistent with its comparatively higher RMSE (1.81 MPa).

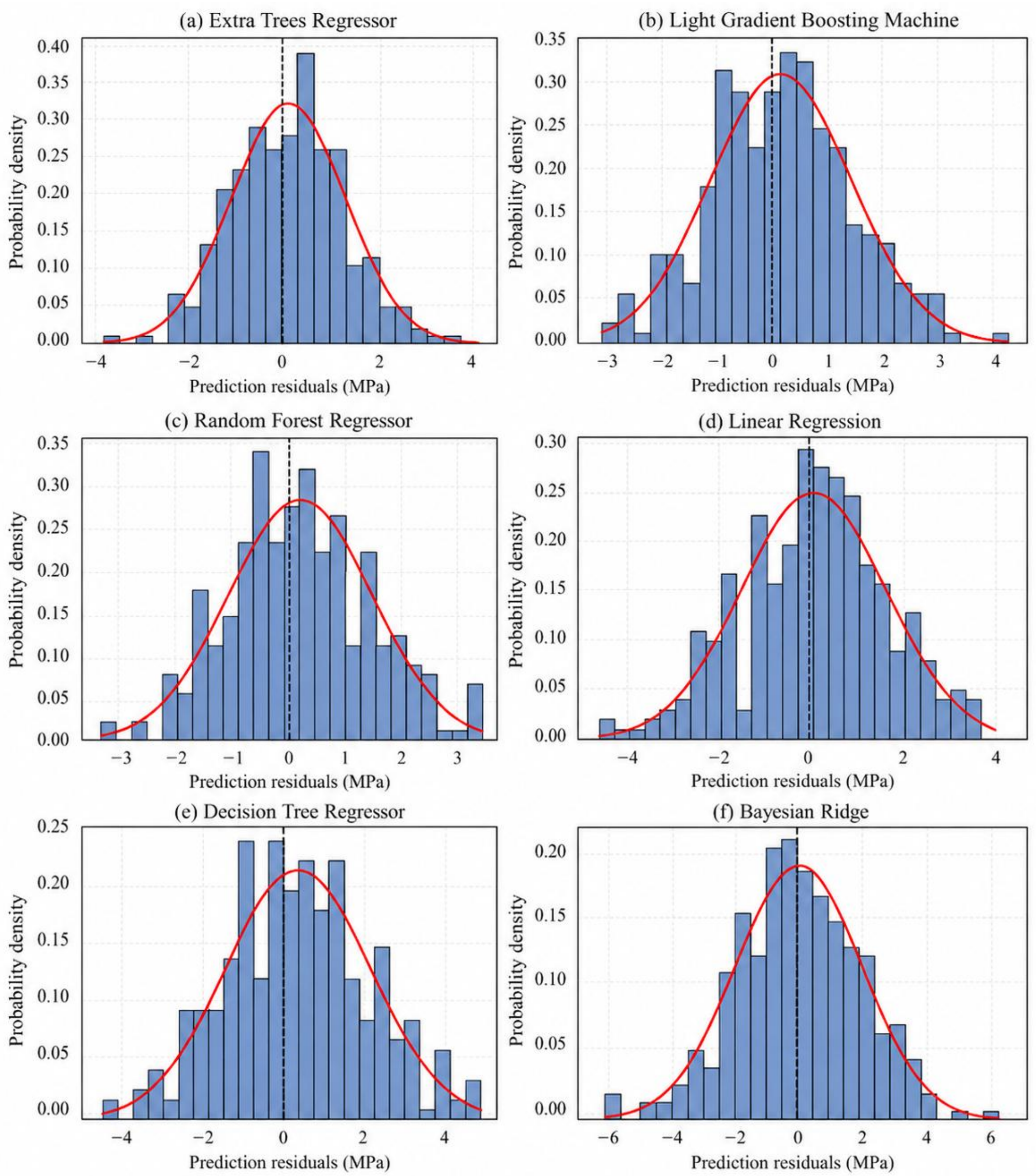


Figure 5. Distribution of prediction residuals obtained using different machine learning models: (a) Extra Trees regressor, (b) Light Gradient Boosting Machine, (c) random forest regressor, (d) linear regression, (e) decision tree regressor, and (f) Bayesian ridge regression.

5.2 Statistical reliability and bias assessment.

Beyond conventional accuracy metrics, statistical reliability was assessed using mean bias error (MBE) and hypothesis testing. The MBE values for all models were close to zero, indicating the absence of systematic overestimation or underestimation of compressive strength. Notably, the Extra Trees Regressor exhibited an MBE of 0.12 MPa, confirming its unbiased prediction capability.

The t-statistic and corresponding p-values further support this observation. For all models, p-values exceeded the 0.05 significance threshold, indicating no statistically significant difference between predicted and experimental compressive strength values. The statistical consistency observed in ensemble models enhances confidence in their applicability for engineering decision-making, where unbiased and reliable predictions are essential (Montgomery et al., 2012).

5.3 Influence of multicollinearity on model performance.

VIF analysis revealed severe multicollinearity among several particle packing related input variables. Fly ash content, coarse aggregate content, fine aggregate ratio, and water-to-binder ratio exhibited extremely high VIF values, confirming strong interdependence among these parameters. Such multicollinearity explains the reduced performance of linear and Bayesian regression models, as coefficient instability and inflated variance compromise predictive reliability.

As shown in Table 3, several particle packing related variables exhibit severe multicollinearity, particularly fly ash content, aggregate fractions, and water to binder ratio, whereas recycled aggregate content remains statistically independent. The recycled aggregate replacement ratio exhibited a VIF value close to unity, indicating statistical independence. This characteristic makes recycled aggregate content a robust predictor in both linear and nonlinear modeling frameworks. The superior performance of tree-based ensemble models observed in this study aligns with previous findings that these algorithms are inherently resilient to multicollinearity and capable of capturing complex variable interactions without requiring explicit feature decorrelation (Breiman, 2001; Li et al., 2022). Part of the observed multicollinearity can also be attributed to inconsistencies in reporting cement types and supplementary cementitious materials across different studies. In particular, the use of blended cements containing fly ash may lead to overlapping representation of binder components, thereby amplifying statistical correlations among input variables.

5.4 SHAP-based interpretation of particle packing indicators.

To determine the relative significance of particle packing indicators and to interpret the predictions of the top-performing model, SHapley Additive exPlanations (SHAP) analysis was performed. The findings show that the most important factor is the percentage of recycled aggregate replacement, which is followed by cement content and water to binder ratio. This ranking highlights the dominant role of aggregate quality, paste availability, and internal void structure in governing compressive strength development in RA-SCC (Tang et al., 2023).

The strong influence of recycled aggregate content can be attributed to its impact on particle packing efficiency and interfacial transition zone characteristics. Recycled aggregates introduce additional porosity and surface roughness due to adhered mortar, which affects both packing density and stress transfer mechanisms (Etxeberria et al., 2007; Poon et al., 2004; H. Zhang et al., 2022). Cement content and water to binder ratio directly control paste volume and hydration products, further influencing void filling and particle connectivity. For the top-performing machine learning model, SHapley Additive exPlanations were used to analyze the contribution of individual particle packing indicators to compressive strength prediction. The SHAP summary plot shows how individual SHAP values are distributed throughout the training dataset, and the feature importance bar plot is created using the final mean absolute SHAP values that were acquired from the trained Extra Trees Regressor. Table 5 provides a summary of the mean absolute SHAP values and associated feature rankings. This consistency between explainable machine learning outcomes and established concrete mechanics enhances confidence in the practical applicability of the proposed framework.

Table 5. SHAP-based feature importance ranking for the best performing model.

Rank	Feature	Mean absolute SHAP value
1	Recycled aggregate content (RA %)	2.476
2	Cement	1.483
3	Water-to-binder ratio (W/B)	1.401
4	Fly ash (FA)	0.728
5	Coarse aggregate (CA)	0.703
6	Aggregate volume fraction (AVF)	0.694
7	Packing index (PI)	0.157
8	Water	0.088
9	Fine aggregate ratio (FAR)	0.08
10	Age	0

Note: *Mean absolute SHAP values represent the average magnitude of each feature's contribution to model predictions. Higher values indicate greater influence on compressive strength. FAR denotes fine aggregate ratio, AVF denotes aggregate volume fraction, PI denotes packing index, and W/B denotes water-to-binder ratio.*

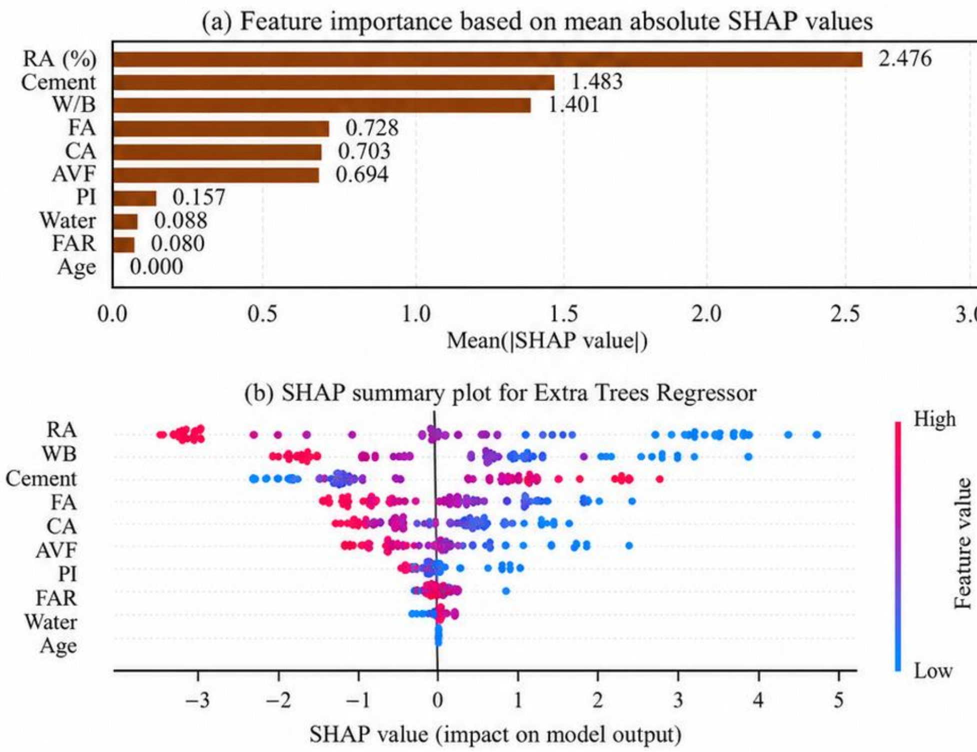


Figure 6. SHAP based interpretation of the Extra Trees Regressor showing (a) feature importance ranked by mean absolute SHAP values and (b) SHAP summary plot illustrating the influence of particle packing related input variables on compressive strength prediction.

Figure 6 presents the SHAP based explainability analysis for the Extra Trees Regressor, providing quantitative insight into the relative contribution of particle packing related variables to compressive strength prediction. The recycled aggregate replacement ratio is the most significant predictor, with the greatest mean absolute SHAP value (2.48), followed by cement content (1.48), and water to binder ratio (1.40), according to the feature importance plot in Fig. 6(a). It should also be noted that the relatively higher importance of recycled aggregate content may be partially influenced by its broader range of variation (0-100%) compared to other input variables. This wider variability increases its statistical contribution within the model and should be considered when interpreting feature importance rankings. These variables directly control aggregate quality, paste availability, and internal void structure, which collectively govern particle packing efficiency in self compacting concrete.

Fly ash content (0.73), coarse aggregate content (0.70), and aggregate volume fraction (0.69) all show moderate contributions, which is indicative of their secondary function in fine-tuning packing density and paste dispersion. In contrast, packing index (0.16), water content (0.09), and fine aggregate ratio (0.08) exhibit relatively limited influence, while curing age shows negligible contribution within the analyzed dataset.

The SHAP summary plot in Fig. 6(b) further illustrates the directional influence of these variables across individual predictions. Higher recycled aggregate content and increased water to binder ratio generally exert a negative effect on compressive strength, whereas higher cement content contributes positively. The SHAP results confirm that the Extra Trees model captures physically meaningful particle packing mechanisms and provide transparent, data driven support for the proposed predictive framework. It should also be emphasized that, due to multicollinearity among binder-related variables, the SHAP values reflect distributed contributions across correlated inputs. Consequently, the relative importance of individual variables should be interpreted in conjunction with domain knowledge rather than as independent causal effects.

Supplementary cementitious material content and aggregate volumetric parameters exhibited moderate contributions, indicating their secondary but non negligible role in refining particle packing and microstructure. Conversely, curing age showed negligible influence within the compiled dataset, suggesting that mix composition parameters dominate strength variation in the selected data range. It is important to critically interpret the relatively low importance of the packing index (PI) and fine aggregate ratio (FAR), despite their conceptual relevance to particle packing behavior. While these parameters are intended to represent packing characteristics, they are derived or secondary indicators that depend on the underlying mix composition variables. As a result, their independent contribution to model predictions is comparatively limited. In contrast to mix design variability, similar findings have been documented in literature-based datasets with a restricted age distribution (Asteris et al., 2020; Fanijo et al., 2023). The SHAP analysis indicates that primary mix design variables such as recycled aggregate content, cement content, and water-to-binder ratio exert a stronger influence on compressive strength. This is because these parameters directly govern paste volume, particle interaction, and void structure, which collectively define packing efficiency. In contrast, PI and FAR capture these effects in an aggregated or indirect manner, leading to lower individual importance in the ML model. This observation does not contradict the particle packing-based framework proposed in this study. Rather, it demonstrates that ML model implicitly capture packing mechanisms through dominant mix design variables, without relying heavily on explicitly defined packing indices. The results suggest that packing behavior is inherently embedded within the relationships among cementitious content, aggregate proportions, and water demand, rather than being governed by a single indicator variable. Therefore, the relatively lower ranking of PI and FAR should be interpreted as an indication that particle packing effects are distributed across multiple interacting variables, rather than being isolated in specific indices. This reinforces the capability of explainable machine learning to capture complex physical mechanisms implicitly, aligning with the core objective of this study.

5.5 Implications for particle packing–oriented mix design.

The combined results of VIF and SHAP analyses show that machine learning may implicitly capture particle packing mechanisms through mix composition variables, even though particle packing density or void ratio was not explicitly determined. The strong alignment between SHAP derived feature importance and established packing theory confirms the physical consistency of the developed model. This implicit representation offers a practical alternative to experimental packing tests, which are often time-consuming and material specific (Cheng et al., 2021; de Larrard, 1999).

From a practical perspective, the results suggest that controlling recycled aggregate content, binder dosage, and water to binder ratio is critical for optimizing compressive strength in RA-SCC. The developed framework provides both predictive capability and interpretative insight, supporting data-driven and sustainable concrete mix design.

6. CONCLUSIONS AND FUTURE RESEARCH DIRECTIONS

6.1 Conclusions.

Through the use of particle packing indicators derived from mix composition characteristics, this study created an explainable machine learning framework for forecasting the compressive strength of RA-SCC. From an engineering perspective, the developed model can assist practitioners in selecting recycled aggregate content and binder proportions that balance sustainability and strength requirements, without resorting to trial-and-error laboratory testing. The following conclusions can be made using a dataset based on literature and thorough statistical analysis:

1. Among the six evaluated models, the Extra Trees Regressor demonstrated the highest predictive accuracy, achieving an R^2 of 0.9724, MAE of 0.79 MPa, RMSE of 1.19 MPa, and MAPE of 2.12%. These findings show that the experimental and projected compressive strength values agree quite well.
2. Ensemble based models, including Extra Trees, Random Forest ($R^2 = 0.968$), and Light Gradient Boosting Machine ($R^2 = 0.965$), consistently outperformed linear and Bayesian regression models. This performance advantage highlights the ability of ensemble learners to capture nonlinear interactions among mix design variables governing particle packing behavior.
3. Linear and Bayesian models exhibited reduced accuracy due to severe multicollinearity among particle packing related parameters. Variance inflation factor analysis confirmed strong interdependence among fly ash content, aggregate fractions, and water to binder ratio, while recycled aggregate replacement ratio remained statistically independent.
4. Analysis of statistical dependability revealed that all models had very little prediction bias. The robustness of the devised framework was supported by the Extra Trees Regressor's mean bias error of 0.12 MPa and hypothesis testing, which revealed no statistically significant difference between predicted and measured strengths ($p > 0.05$).
5. SHapley Additive exPlanations analysis identified recycled aggregate replacement ratio as the most influential parameter, followed by cement content and water to binder ratio. This ranking is physically consistent with particle packing theory, as aggregate quality, paste availability, and internal void structure collectively govern compressive strength development.

6. The significant agreement between SHAP-based feature importance and well-established packing principles shows that machine learning may implicitly capture particle packing mechanisms through mix composition variables, even though particle packing density or void ratio was not explicitly estimated.

The suggested framework supports sustainable concrete design and performance evaluation by offering a precise, statistically sound, and physically interpretable method for RA-SCC compressive strength prediction. The findings demonstrate that explainable machine learning can serve as a reliable decision-support tool for sustainable RA-SCC mix design in both research and practice. The use of a dataset consisting of 365 mixtures compiled from 102 independent studies further strengthens the statistical reliability and practical applicability of the proposed predictive framework.

6.2 Future research directions.

Although the current work shows that explainable machine learning is a useful tool for predicting compressive strength, there are several areas that could use more investigation:

1. Future studies may incorporate experimentally measured particle packing density or void ratio as explicit input variables to strengthen the mechanistic linkage between machine learning predictions and physical packing behavior.
2. To enhance model generality across various building scenarios, the dataset might be enlarged to encompass a greater range of curing ages, recycled aggregate grades, and self-compacting concrete rheological characteristics.
3. Hybrid modeling approaches combining particle packing theory with data-driven machine learning frameworks could be explored to further enhance prediction accuracy and interpretability.
4. Extension of the proposed methodology to predict durability-related properties, such as permeability, shrinkage, and long-term strength development, would broaden its applicability in sustainable infrastructure design.
5. Lastly, explainable machine learning models can be used with uncertainty quantification techniques to offer prediction confidence boundaries, facilitating risk-informed engineering practice.
6. Future research should focus on validating the proposed machine learning framework using controlled experimental datasets obtained from single research programs. Such studies would enable more precise assessment of model performance under consistent material and testing conditions and support the development of project-specific predictive tools.
7. In addition, future studies should incorporate datasets covering multiple curing ages to enable time-dependent strength prediction. This is particularly important for concrete systems incorporating supplementary cementitious materials such as fly ash, where long-term strength development extends beyond the conventional 28-day period.

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