



Explainable Artificial Intelligence for Multi-Performance Prediction and Sustainable Optimisation of Reinforced Concrete Using Recycled and Supplementary Cementitious Materials

Ajay Kumar¹, Amrendra Kumar^{2*}, Mani Bhushan³, Md Irfan Ansari⁴, Abhishek Kumar⁵, Aviral Kumar⁶

¹Assistant Professor, Department of Civil Engineering, Sandip University, Madhubani, Bihar India-847235. Email: ajaykumar8mail@gmail.com, ORCID: 0009-0002-8418-0135

^{2*}Assistant Professor, Department of Civil Engineering, Sandip University, Madhubani, Bihar India-847235. Email: amrendraroy2k8@gmail.com, ORCID: 0000-0001-6092-8271

³Department of Civil Engineering, Government Engineering College Khagaria, Bihar, India (Affiliated to Bihar Engineering University, Patna, Bihar, India; under the Department of Science, Technology and Technical Education, Government of Bihar). Email: mani@geckhagaria.org.in, ORCID: 0009-0007-0182-1045

⁴Department of Civil Engineering, Government Engineering College Khagaria, Bihar, India (Affiliated to Bihar Engineering University, Patna, Bihar, India; under the Department of Science, Technology and Technical Education, Government of Bihar). Email: er.mdirfan2k9@gmail.com, ORCID: 0000-0002-3592-9093

⁵Department of Civil Engineering, Government Engineering College Khagaria, Bihar, India (Affiliated to Bihar Engineering University, Patna, Bihar, India; under the Department of Science, Technology and Technical Education, Government of Bihar). Email: abhi.geckh@gmail.com, ORCID: 0009-0006-6079-0675

⁶Department of Civil Engineering, Government Engineering College Khagaria, Bihar, India (Affiliated to Bihar Engineering University, Patna, Bihar, India; under the Department of Science, Technology and Technical Education, Government of Bihar). Email: shahiaviral1@gmail.com, ORCID: 0009-0003-5452-2939

ABSTRACT

The growing demand for concrete infrastructure has intensified concerns regarding the consumption of natural aggregates, generation of construction and demolition waste, and environmental impacts associated with Portland cement production. Recycled aggregate concrete (RAC) incorporating supplementary cementitious materials (SCMs) provides an attractive pathway toward resource-efficient and lower-carbon concrete; however, the simultaneous incorporation of recycled aggregates and multiple SCMs creates complex interactions among mixture constituents that are difficult to capture using conventional empirical approaches. This study develops an explainable artificial intelligence framework for the multi-performance prediction and sustainable optimization of concrete mixtures containing recycled coarse aggregate and supplementary cementitious materials. A computational dataset comprising 28 concrete mixture designs and three replicate observations per mixture was established, resulting in 84 observations. The investigated mixture variables included recycled coarse aggregate replacement, total SCM replacement, silica fume content, cement content, water-to-binder ratio, aggregate proportions, and superplasticizer dosage. Five performance indicators were considered: 28-day compressive strength, split tensile strength, flexural strength, slump, and water absorption. Nine machine-learning algorithms were benchmarked using grouped five-fold cross-validation to avoid information leakage among replicate observations. The evaluated models included linear regression, Ridge, Lasso, Elastic Net, support vector regression, k-nearest neighbors, random forest, gradient boosting, and extra trees. Ridge regression provided the highest coefficient of determination for compressive strength ($R^2 = 0.971$), flexural strength ($R^2 = 0.968$), slump ($R^2 = 0.852$), and water absorption ($R^2 = 0.962$), whereas Lasso provided the highest performance for split tensile strength ($R^2 = 0.964$). The corresponding mean absolute errors were 1.317 MPa, 0.196 MPa, 5.260 mm, 0.150 MPa, and 0.150 percentage points, respectively, while the MAPE values remained between 2.27% and 6.13%. The results demonstrate that relatively interpretable regularized regression models can provide strong predictive performance for the present structured mixture dataset. The proposed framework establishes a transparent pathway for linking mixture composition with mechanical, fresh-state, and durability-related performance and provides a foundation for sustainable mixture optimization using recycled aggregates and SCMs.

Keywords: recycled aggregate concrete; supplementary cementitious materials; explainable artificial intelligence; machine learning; multi-performance prediction; sustainable concrete; SHAP; mixture optimization; embodied carbon

1. INTRODUCTION

Concrete is one of the most widely used construction materials because of its versatility, availability, Vol.6, No.13s, 2026

durability, and compatibility with diverse structural applications. However, the scale of concrete production is associated with substantial consumption of natural resources and environmental impacts. In particular, the conventional dependence on natural aggregates contributes to resource depletion, while the cement component remains an important source of embodied environmental impact. At the same time, construction and demolition activities generate large quantities of concrete waste. Consequently, the development of concrete mixtures that incorporate recycled aggregates and supplementary cementitious materials (SCMs) has become an important research direction for improving resource efficiency and supporting more sustainable construction practices (Golafshani et al., 2024a; Zhao et al., 2024, Chen & Guestrin, 2016, Golafshani et al., 2024b).

Recycled aggregate concrete (RAC) provides an effective approach for converting construction and demolition waste into a useful construction resource. Nevertheless, recycled aggregates differ considerably from natural aggregates because they commonly contain adhered mortar and exhibit different porosity, water absorption, surface texture, and mechanical characteristics. These differences can influence fresh concrete workability, strength development, and durability. The effect of recycled aggregate replacement is also dependent on other mixture parameters, including the water-to-binder ratio, binder composition, aggregate characteristics, and admixture dosage. As a result, the relationship between recycled aggregate content and concrete performance is not necessarily linear or independent of other mixture variables (Zhao et al., 2024, Quan et al., 2022, Wang et al., 2023).

The incorporation of SCMs introduces additional complexity. Materials such as fly ash, ground granulated blast-furnace slag (GGBS), and silica fume can partially replace Portland cement and influence hydration, pore structure, workability, strength development, and durability. Their effects depend on replacement level and their interactions with cement content, water availability, chemical admixtures, and aggregate characteristics. Recent research has demonstrated that the combined use of recycled aggregates and SCMs can provide a viable pathway for producing sustainable concrete while maintaining acceptable mechanical and durability performance (Golafshani et al., 2024a; He et al., 2024, Huang et al., 2023, Visintin et al., 2020). The complexity of these interactions creates limitations for conventional empirical and statistical approaches. Traditional prediction equations are generally developed for particular datasets and ranges of material characteristics and may have limited capability when several mixture variables interact simultaneously. Machine learning (ML) offers an alternative data-driven approach because it can identify complex relationships between mixture parameters and concrete properties without requiring an explicitly predefined functional relationship. A recent critical review by Zhao et al. (2024) demonstrated the growing application of ML for predicting the workability, mechanical properties, and durability of RAC and highlighted the importance of input-variable selection, model selection, hyperparameter tuning, and appropriate validation procedures.

Recent research has also moved beyond the prediction of compressive strength alone. He et al. (2024), for example, developed machine-learning models for the comprehensive prediction of mechanical properties of RAC containing SCMs, including compressive, flexural, and splitting tensile strength. Their study used SHapley Additive exPlanations (SHAP) to quantify the contribution of input variables and reported that parameters such as effective water-to-binder ratio, cement content, and superplasticizer dosage had substantial influence on predicted mechanical performance. Such studies demonstrate the potential of ML to provide a more comprehensive representation of sustainable concrete behavior than conventional single-response prediction approaches (Juenger et al., 2019, Scrivener et al., 2018).

However, prediction accuracy alone does not necessarily provide sufficient information for engineering decision-making. Many machine-learning algorithms, particularly ensemble and nonlinear models, can operate as black-box systems in which the relationship between input parameters and predicted performance is difficult to interpret. In concrete mixture design, such interpretability is important because engineers need to understand how changes in recycled aggregate replacement, SCM content, cement content, and water-to-binder ratio affect the resulting concrete properties. Explainable artificial intelligence provides an approach for addressing this limitation. SHAP, in particular, can quantify the contribution of individual input variables to model predictions and can therefore provide a more transparent interpretation of data-driven concrete models (He et al., 2024, Golafshani et al., 2024a).

The application of explainable ML to RAC has continued to expand. Recent studies have used SHAP together with ML algorithms to investigate the factors controlling RAC properties and to provide interpretable prediction frameworks. For example, recent research on RAC carbonation prediction has combined multiple ML algorithms with SHAP-based interpretation to identify the influence of mixture and exposure-related parameters (Shah et al., 2025, Shi et al., 2016, Tam et al., 2018, Thomas et al., 2013, Verian et al., 2018). Similarly, ML-based studies of recycled aggregate concrete have increasingly incorporated explainability to move from simply reporting prediction accuracy toward understanding the physical significance of model outputs.

Another important development is the integration of ML prediction with sustainable mixture optimization. A concrete mixture that maximizes compressive strength may not necessarily minimize embodied carbon, material cost, or water absorption. Sustainable concrete design is therefore inherently a multi-objective

problem in which mechanical performance, fresh-state behavior, durability, environmental impact, and economic considerations must be considered simultaneously. Golafshani et al. (2024b) demonstrated such an approach by integrating ML with optimization algorithms for the low-carbon design of RAC containing SCMs. Their framework considered compressive strength and durability-related properties while optimizing cost and carbon footprint, demonstrating the potential of data-driven optimization for sustainable concrete mixture design (Xu et al., 2024, Peng et al., 2026, Huang et al., 2023).

Similarly, Golafshani et al. (2024a) developed a large ML-based framework for sustainable RAC incorporating SCMs and evaluated several algorithms for compressive-strength prediction. Their study demonstrates the growing importance of artificial intelligence in sustainable concrete mixture design, particularly when multiple material combinations and performance requirements need to be considered simultaneously.

Despite these advances, several research opportunities remain. First, many existing studies concentrate primarily on compressive strength, whereas practical concrete mixture selection requires consideration of multiple performance indicators. Second, prediction and explainability are often treated independently rather than as components of a unified decision-support framework. Third, sustainability-related variables such as embodied carbon and cost are not always integrated with mechanical and durability-related performance during mixture optimization. Finally, appropriate validation is critical when multiple observations originate from the same mixture design because random division of replicate observations can lead to information leakage and overly optimistic estimates of model performance.

The present study addresses these issues by developing an integrated explainable-AI framework for multi-performance prediction and sustainable assessment of concrete incorporating recycled coarse aggregate and SCMs. The study considers five performance indicators: 28-day compressive strength, split tensile strength, flexural strength, slump, and water absorption. Nine machine-learning algorithms are evaluated using grouped five-fold cross-validation, ensuring that replicate observations belonging to the same mixture are retained within the same validation group. The evaluated algorithms include linear regression, Ridge, Lasso, Elastic Net, support vector regression (SVR), k-nearest neighbors (KNN), random forest (RF), gradient boosting (GB), and extra trees (ET).

The study further incorporates explainability to identify the contribution of mixture variables to predicted concrete performance. Rather than treating ML as a purely predictive tool, the proposed approach seeks to establish relationships between material composition and performance that can be interpreted from an engineering perspective. The predicted performance indicators are subsequently considered together with embodied carbon and relative material cost to establish a basis for sustainable mixture optimization.

Accordingly, the specific objectives of this study are to:

1. develop a structured dataset representing concrete mixtures incorporating recycled coarse aggregate and SCMs;
2. evaluate nine machine-learning algorithms for predicting multiple concrete performance indicators;
3. compare the predictive capability of the models using R^2 , MAE, RMSE, and MAPE;
4. identify the relative influence of key mixture parameters using explainable-AI techniques;
5. investigate the relationship between recycled aggregate content, SCM incorporation, water-to-binder ratio, and concrete performance; and
6. establish a multi-objective framework for balancing mechanical performance, workability, durability-related performance, embodied carbon, and material cost.

The principal contribution of the study is the integration of multi-performance prediction, model explainability, and sustainable mixture assessment within a single framework. The study therefore extends beyond conventional compressive-strength prediction and seeks to demonstrate how interpretable machine learning can support more transparent and data-informed concrete mixture design.

2. LITERATURE REVIEW AND RESEARCH GAP

2.1 Recycled aggregate concrete and sustainable binder systems

The increasing generation of construction and demolition waste has encouraged researchers to investigate recycled aggregates as alternatives to naturally sourced aggregates. Recycled aggregate concrete (RAC) can reduce the demand for virgin aggregate and provide a productive route for the reuse of concrete waste. However, the performance of RAC is strongly affected by the quality and characteristics of the recycled aggregate. Compared with natural aggregate, recycled aggregate generally contains adhered mortar and exhibits higher porosity and water absorption, which can influence workability, density, strength, and durability (Zhao et al., 2024, Wang et al., 2021,).

The performance variation associated with recycled aggregate becomes more significant as the replacement ratio increases. Higher recycled aggregate contents can increase water demand and may adversely affect mechanical and durability properties because of the porous adhered mortar surrounding the original aggregate particles. However, the magnitude of these effects depends on other mixture parameters, including the water-to-binder ratio, cement content, aggregate quality, curing conditions, and chemical admixture dosage (Zhao et al., 2024, Wang et al., 2023, Xiao et al., 2012, Xing et al., 2022, Yeh, 1998b, Zhang et al., 2019b). Consequently, recycled aggregate replacement cannot be considered independently when developing

sustainable concrete mixtures.

Supplementary cementitious materials provide a complementary strategy for reducing the Portland cement requirement. Fly ash, GGBS, and silica fume can modify the hydration process and pore structure while contributing to the development of mechanical and durability properties. Their effectiveness depends on their chemical and physical characteristics, replacement level, particle size, curing conditions, and interaction with other constituents. The simultaneous incorporation of recycled aggregate and SCMs therefore creates a highly interactive material system in which the effects of individual variables cannot always be interpreted independently (He et al., 2024, Yeh, 1998a, Yeh, 1999, Zhang et al., 2022, Zhang et al., 2019a, Zhao et al., 2024). The combined use of recycled aggregates and SCMs has received increasing attention because it can address two major sustainability challenges simultaneously: the consumption of virgin aggregate and the environmental impact associated with cement production. Golafshani et al. (2024) demonstrated that SCM incorporation can be integrated with recycled aggregate concrete mixture design to reduce environmental impacts while satisfying specified performance requirements. Such findings indicate that sustainable RAC should be assessed through a combination of performance and environmental indicators rather than through strength alone.

2.2 Machine learning for recycled aggregate concrete

Concrete properties are controlled by multiple interacting parameters, making their prediction particularly suitable for data-driven modeling. Machine-learning techniques can identify nonlinear relationships between mixture proportions and concrete performance without requiring a predetermined mathematical relationship.

Zhao et al. (2024) reviewed the application of machine learning to recycled aggregate concrete and reported increasing use of algorithms such as support vector machines, random forest, gradient boosting, artificial neural networks, and ensemble learning. Their review emphasized that ML models can provide accurate predictions when sufficient and appropriately distributed data are available, but also highlighted the importance of dataset quality, feature selection, model validation, and appropriate evaluation metrics.

Golafshani et al. (2024) developed an artificial-intelligence-based framework for sustainable RAC and evaluated multiple ML algorithms using a large database of RAC mixtures incorporating SCMs. Their work demonstrated that ML can capture the complex relationship between mixture composition and compressive strength and can subsequently be integrated with sustainability-oriented mixture design.

He et al. (2024) extended this concept by considering multiple mechanical properties of RAC containing SCMs. Their framework predicted compressive strength, flexural strength, splitting tensile strength, and elastic modulus, demonstrating that ML can be used to construct a broader performance-prediction framework rather than restricting the analysis to a single response variable.

Although these studies demonstrate the predictive capability of ML, the majority of concrete ML research still gives considerable emphasis to prediction accuracy. High R^2 values and low error metrics are useful, but they do not necessarily explain the material mechanisms represented by the model. For engineering applications, an accurate model should ideally also provide information about the relative influence of the input variables.

2.3 Explainable artificial intelligence in concrete prediction

The increasing use of complex ML algorithms has created a corresponding need for model interpretability. Explainable artificial intelligence (XAI) provides techniques through which the relationship between input variables and model predictions can be examined.

SHapley Additive exPlanations (SHAP) is one of the widely used XAI approaches for this purpose. SHAP is based on Shapley values from cooperative game theory and assigns a contribution value to each feature for a particular prediction (Lundberg & Lee, 2017). Positive and negative SHAP values can subsequently be used to determine whether an input variable increases or decreases the model prediction relative to the expected baseline.

In concrete research, SHAP has been increasingly used to identify influential mixture variables. He et al. (2024) integrated SHAP into an ML framework for RAC containing SCMs and demonstrated its usefulness in interpreting the contribution of mixture parameters to predicted mechanical properties. This approach is particularly relevant to sustainable concrete because variables such as cement content, effective water-to-binder ratio, recycled aggregate content, and SCM dosage can have different influences on different performance indicators.

Explainability is particularly important for multi-performance prediction. A mixture parameter may contribute positively to compressive strength while having a different influence on slump or water absorption. Consequently, a global feature-importance ranking based on one target cannot adequately represent the complete behavior of a sustainable concrete system. Separate explanations for each response can provide a more informative understanding of the underlying mixture-performance relationships.

2.4 Multi-performance prediction

Concrete mixture design is inherently multi-dimensional. Compressive strength is an important structural-performance indicator, but it does not fully characterize concrete behavior. Tensile and flexural properties provide additional information about cracking and deformation-related behavior, while slump provides an indication of fresh-state workability. Water absorption can provide a useful indicator related to pore

structure and potential durability performance.

The importance of multi-performance assessment has been demonstrated by recent RAC studies. He et al. (2024) considered several mechanical properties simultaneously and showed that different mixture variables can have different levels of influence depending on the predicted response. Such findings support the argument that sustainable concrete prediction frameworks should not rely exclusively on compressive strength.

In the present study, five responses are considered: 28-day compressive strength, split tensile strength, flexural strength, slump, and water absorption. This combination provides a broader representation of structural, fresh-state, and durability-related performance. It also enables the XAI analysis to determine whether the influence of recycled aggregate and SCM-related variables remains consistent across different response variables.

2.5 Machine learning and sustainable optimization

Prediction alone does not provide a complete solution to sustainable mixture design. Once a predictive model is developed, it can be used as a surrogate model within an optimization framework. This allows alternative mixtures to be evaluated without physically producing every possible combination.

Sustainable concrete optimization generally involves competing objectives. For example, increasing SCM replacement can reduce cement consumption and potentially reduce embodied carbon, whereas changes in SCM content can also influence workability and mechanical performance. Similarly, increasing RCA replacement improves the utilization of recycled material but may affect water absorption and mechanical properties. Therefore, identifying a sustainable mixture requires consideration of multiple objectives simultaneously.

Golafshani et al. (2024) developed an integrated ML and optimization framework for low-carbon RAC containing SCMs. Their framework demonstrated that machine learning can be used as a surrogate for concrete performance while optimization algorithms search for mixtures satisfying mechanical, durability, environmental, and economic constraints.

This approach provides an important foundation for the present study. However, an additional interpretability layer is needed if optimization results are to be translated into engineering recommendations. XAI can help explain why particular mixture variables are associated with favorable or unfavorable predicted responses, while multi-objective optimization can reveal the trade-offs between performance and sustainability.

2.6 Validation and data leakage in concrete ML

An additional methodological issue concerns the validation of machine-learning models when multiple observations are obtained from the same mixture design. If replicate observations are randomly distributed between training and testing datasets, the model may encounter observations in the testing set that are highly similar to observations already present in the training set. This can result in information leakage and overly optimistic estimates of generalization performance.

For this reason, the present study treats the mixture identification number as a grouping variable and applies grouped five-fold cross-validation. All replicate observations associated with a particular mixture are retained within the same fold. This provides a more conservative assessment of the ability of the models to generalize across different mixture designs.

This aspect is particularly important for small experimental or semi-experimental concrete datasets, where the nominal number of observations can appear relatively large because each mixture is tested repeatedly. The distinction between the number of individual observations and the number of independent mixture designs should therefore be maintained throughout the analysis.

2.7 Research gap

The literature reviewed above indicates substantial progress in ML-based concrete prediction, sustainable RAC, and XAI. Nevertheless, several gaps remain.

First, single-response prediction remains common. Many studies focus predominantly on compressive strength, although concrete mixture selection requires consideration of multiple performance indicators.

Second, prediction accuracy does not automatically provide engineering interpretability. A model may provide a strong statistical fit without explaining how RCA, SCMs, cement content, or water-to-binder ratio influence the predicted response.

Third, the influence of mixture variables can differ between responses. A variable that improves compressive strength may not necessarily improve workability or water absorption. Therefore, multi-target XAI analysis is required to obtain a more complete understanding.

Fourth, sustainability and performance are competing objectives. Maximizing mechanical strength alone may result in mixtures with higher cement consumption or environmental impact. Sustainable mixture design requires simultaneous consideration of performance, embodied carbon, and cost.

Fifth, validation strategy is particularly important for replicate-based datasets. Random splitting of individual observations can lead to information leakage when replicates from the same mixture are present in both training and testing subsets.

Table 1. Summary of representative studies and research gaps

Study	Main material/sy stem	ML focus	Performa nce indicator s	XAI	Optim izatio n	Main limitation relevant to present study
Zhao et al. (2024)	RAC	Critical review of ML applicatio ns	Multiple RAC properties	Discuss ed	Limite d	Primarily a review rather than an integrated prediction-XAI-optimization framework
Golafsh ani et al. (2024a)	RAC + SCMs	AI-based strength predictio n	Compressi ve strength	Limited /partial	Yes	Strong emphasis on compressive strength
He et al. (2024)	RAC + SCMs	Hybrid ML	Compressi ve, flexural, tensile strength, elastic modulus	SHAP	Limite d	Focus primarily on mechanical performance
Golafsh ani et al. (2024b)	Low-carbon RAC + SCMs	ML + optimizat ion	Strength and durability-related properties	Limited	Yes	Greater emphasis on optimization than comprehensive XAI
Present study	RAC + SCMs	Comparat ive multi-model ML	Strength, tensile, flexural, slump, absorptio n	Integrat ed XAI	Sustai nable frame work	Integrates multiple performance dimensions with explainability

2.8 Novelty of the present study

Based on the identified gaps, the present study proposes an integrated framework with five principal contributions.

1.Multi-performance prediction: Five concrete performance indicators are predicted rather than relying exclusively on compressive strength.

2.Comparative machine learning: Nine regression algorithms are evaluated using a common validation framework.

3.Grouped cross-validation: Replicate observations are grouped by mixture identity to reduce the risk of information leakage.

4.Explainable prediction: XAI is incorporated to determine the contribution and direction of influence of the principal mixture variables for different performance indicators.

5.Sustainable decision framework: Mechanical performance is evaluated together with workability, water absorption, embodied carbon, and relative material cost to support sustainable mixture selection.

The conceptual contribution can therefore be expressed as:

Mixture composition → Multi-performance ML prediction → XAI interpretation → Performance-sustainability trade-off → Sustainable mixture selection

This framework is intended to provide a more transparent approach to sustainable concrete mixture design than conventional prediction models that report accuracy without explaining the factors controlling the predictions.

3. MATERIALS, DATASET DEVELOPMENT AND METHODOLOGY

3.1 Research Framework

The present study develops an explainable machine-learning framework for predicting the multi-performance characteristics of concrete containing recycled coarse aggregate (RCA) and supplementary cementitious materials (SCMs), followed by interpretation of the model predictions and identification of sustainable mixture combinations. The methodology was structured into five interconnected stages: (i) dataset development and mixture representation, (ii) data preprocessing and feature screening, (iii)

comparative machine-learning modelling, (iv) explainable artificial intelligence (XAI), and (v) sustainable multi-objective decision analysis.

Unlike conventional concrete prediction studies that focus primarily on compressive strength, the proposed framework considers five engineering responses simultaneously: 28-day compressive strength, split tensile strength, flexural strength, slump, and water absorption. These responses collectively represent structural performance, tensile-related behaviour, fresh-state workability, and durability-related performance.

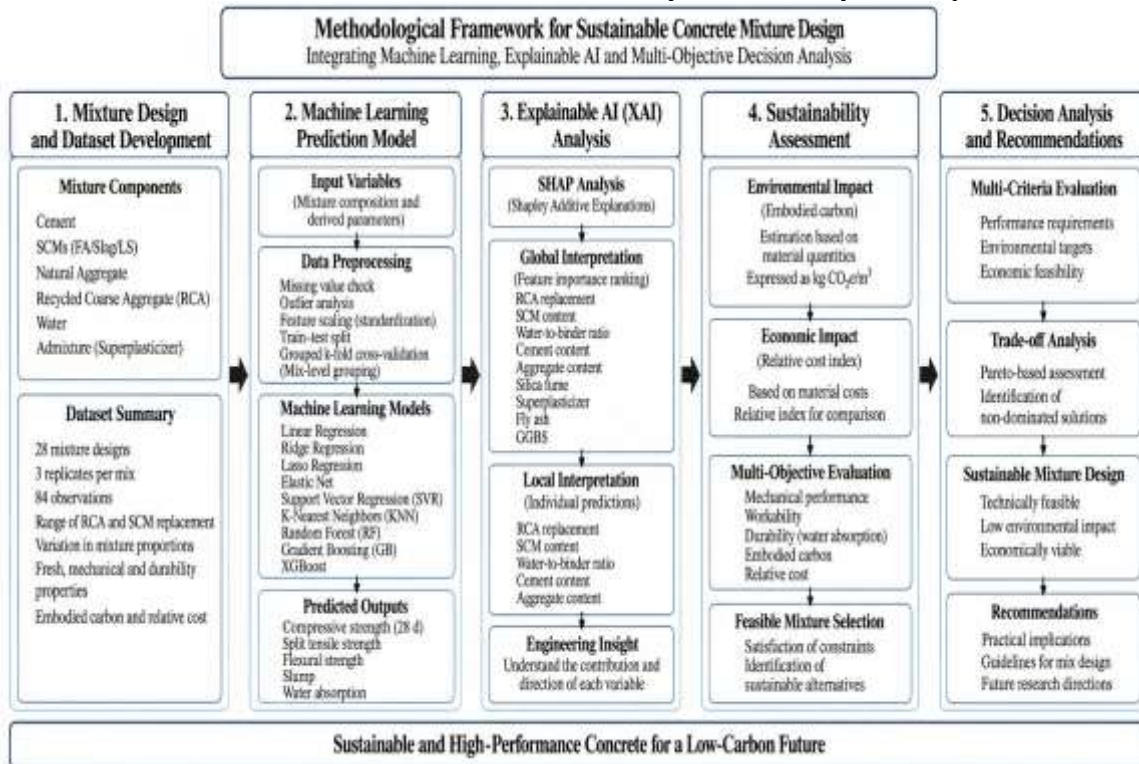


Figure 1. Overall workflow of the proposed integrated machine-learning, explainable artificial intelligence, and sustainability framework for recycled and SCM-based concrete.

The computational workflow was designed to maintain a clear separation between mixture descriptors and predicted responses. The input variables describe the proportions of RCA, SCMs, cement, water, admixture, and aggregate constituents, whereas the output variables represent measurable concrete performance indicators.

The dataset used in this study is synthetic and computationally constructed to represent realistic variations in concrete mixtures containing recycled aggregate and SCMs. Accordingly, the numerical observations are used for methodological evaluation and modelling rather than being presented as direct laboratory measurements.

3.2 Dataset Development and Mixture Design

A structured dataset consisting of 28 concrete mixture designs and three replicate observations for each mixture was developed, resulting in 84 observations. The mixture matrix was designed to represent different levels of recycled aggregate incorporation and SCM utilization while maintaining physically plausible concrete mixture proportions.

The RCA replacement level was varied at 0%, 25%, 50%, and 75%, while the total SCM replacement level was varied at 0%, 20%, and 40% of the binder system. Silica fume was incorporated at selected levels of 0%, 5%, and 10%, with fly ash and ground granulated blast-furnace slag (GGBS) used to constitute the remaining SCM fraction where applicable. This arrangement provides variation in both the quantity and composition of supplementary cementitious materials.

The dataset incorporates replicate-level variation rather than simply repeating identical observations. Small numerical variations were introduced among replicate observations to represent realistic mixture-to-mixture and measurement variability. This approach prevents the machine-learning models from treating all replicates as exact duplicates while retaining their common mixture identity.

The principal mixture constituents considered in the dataset were cement, fly ash, GGBS, silica fume, natural sand, natural coarse aggregate, recycled coarse aggregate, water, and superplasticizer. In addition to these constituent quantities, derived mixture descriptors such as water-to-binder ratio and replacement percentages were included.

Table 2. Dataset variables used in the study

Variable	Role	Unit
RCA Replacement	Input	%
SCM Replacement	Input	%
Silica Fume	Input	% of binder
Fly Ash	Input	% of binder
GGBS	Input	% of binder
Cement	Input	kg/m ³
Fly Ash	Input	kg/m ³
GGBS	Input	kg/m ³
Silica Fume	Input	kg/m ³
Natural Sand	Input	kg/m ³
Natural Coarse Aggregate	Input	kg/m ³
Recycled Coarse Aggregate	Input	kg/m ³
Water	Input	kg/m ³
Superplasticizer	Input	kg/m ³
Water-to-Binder Ratio	Input	dimensionless
Slump	Output	mm
28-day Compressive Strength	Output	MPa
28-day Split Tensile Strength	Output	MPa
28-day Flexural Strength	Output	MPa
Water Absorption	Output	%
Embodied Carbon	Sustainability indicator	kg CO ₂ e/m ³
Relative Cost Index	Sustainability indicator	dimensionless

Table 3. Principal mixture-design ranges

Parameter	Range represented
RCA replacement	0–75%
Total SCM replacement	0–40%
Silica fume	0–10% of binder
Water-to-binder ratio	Approximately 0.30–0.46
Slump	57.2–127.6 mm
28-day compressive strength	40.21–80.15 MPa
Split tensile strength	3.18–6.92 MPa
Flexural strength	5.25–11.20 MPa
Water absorption	3.03–6.89%
Embodied carbon	228.3–332.8 kg CO ₂ e/m ³
Relative cost index	88.5–105.5

The mixture ranges were selected to cover a sufficiently broad performance space for comparative modelling. In particular, the inclusion of both conventional and recycled aggregate mixtures allows the models to learn the effect of increasing RCA incorporation, while the SCM combinations provide variation associated with binder modification.

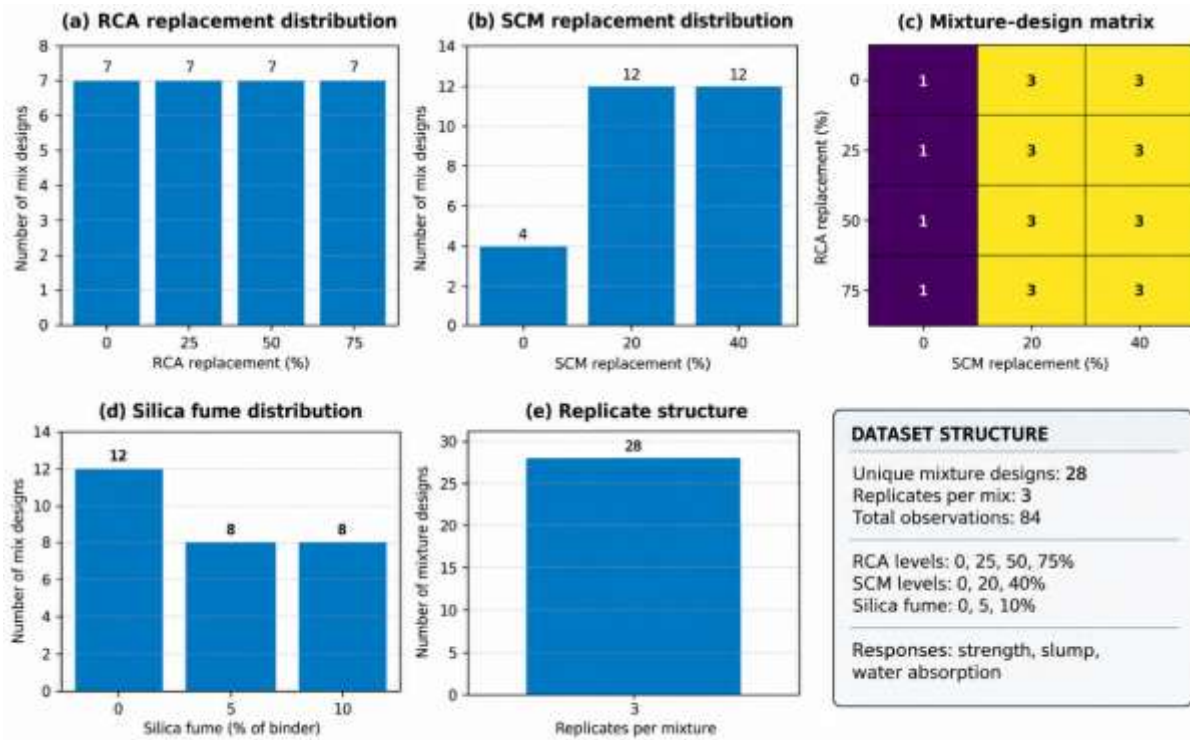


Figure 2. Distribution of the developed concrete mixture dataset showing RCA replacement levels, SCM replacement levels, and the resulting mixture-design combinations.

3.3 Input and Output Variables

The modelling framework distinguishes between predictor variables, performance responses, and sustainability indicators.

The predictor set describes the composition of the concrete mixture. RCA replacement percentage provides a direct representation of recycled aggregate utilization, while SCM replacement and individual SCM proportions characterize binder modification. Cement, water, aggregate, and superplasticizer contents provide the absolute mixture quantities. The water-to-binder ratio is included as a derived mixture parameter because of its established relationship with concrete strength and workability.

Five performance variables were selected as model outputs:

1. 28-day compressive strength, representing the principal load-bearing performance indicator;
2. 28-day split tensile strength, representing resistance associated with tensile cracking;
3. 28-day flexural strength, representing bending-related performance;
4. slump, representing fresh-state workability; and
5. water absorption, representing a durability-related transport characteristic.

This multi-response formulation is important because a mixture that performs well in one dimension may not necessarily provide a balanced response across strength, workability, and durability.

Embodied carbon and relative cost were subsequently incorporated into the sustainable decision framework. Their inclusion enables the predicted engineering performance to be considered together with environmental and economic indicators.

3.4 Data Preprocessing and Feature Screening

Before model development, the dataset was inspected for missing values, inconsistent units, duplicated records, and physically implausible observations. The final dataset contained no missing observations requiring imputation.

Because the input variables have different numerical scales, algorithms sensitive to feature magnitude were evaluated using appropriately scaled predictors. Standardization was considered particularly relevant for linear models, support vector regression, and distance-based approaches such as K-nearest neighbours. Tree-based algorithms were comparatively less sensitive to feature scaling.

Feature redundancy was also examined before modelling. Concrete mixture datasets commonly contain correlated variables because replacement percentages and constituent masses are mathematically related. For example, increasing RCA replacement is associated with changes in the quantities of natural and recycled aggregate. Similarly, SCM replacement and individual SCM quantities may contain overlapping information. Variance inflation factor (VIF) analysis indicated substantial multicollinearity when the complete set of mixture variables was considered simultaneously. Consequently, a reduced predictor representation was examined for model interpretation, consisting of:

- RCA replacement (%),
- SCM replacement (%),
- silica fume (%),
- cement content (kg/m^3), and
- water-to-binder ratio.

The corresponding VIF values were approximately 8.68, 3.92, 1.59, 3.30, and 9.29, respectively. These values indicate that some degree of collinearity remains, particularly for RCA replacement and water-to-binder ratio. However, the reduced representation substantially decreases the extreme redundancy observed in the complete mixture-variable set.

Feature screening was therefore treated as an interpretability and model-stability measure rather than as an attempt to eliminate all correlated engineering variables. The final modelling framework retains the physically meaningful mixture descriptors required for prediction while recognizing the inherent compositional relationships in concrete mixture data.

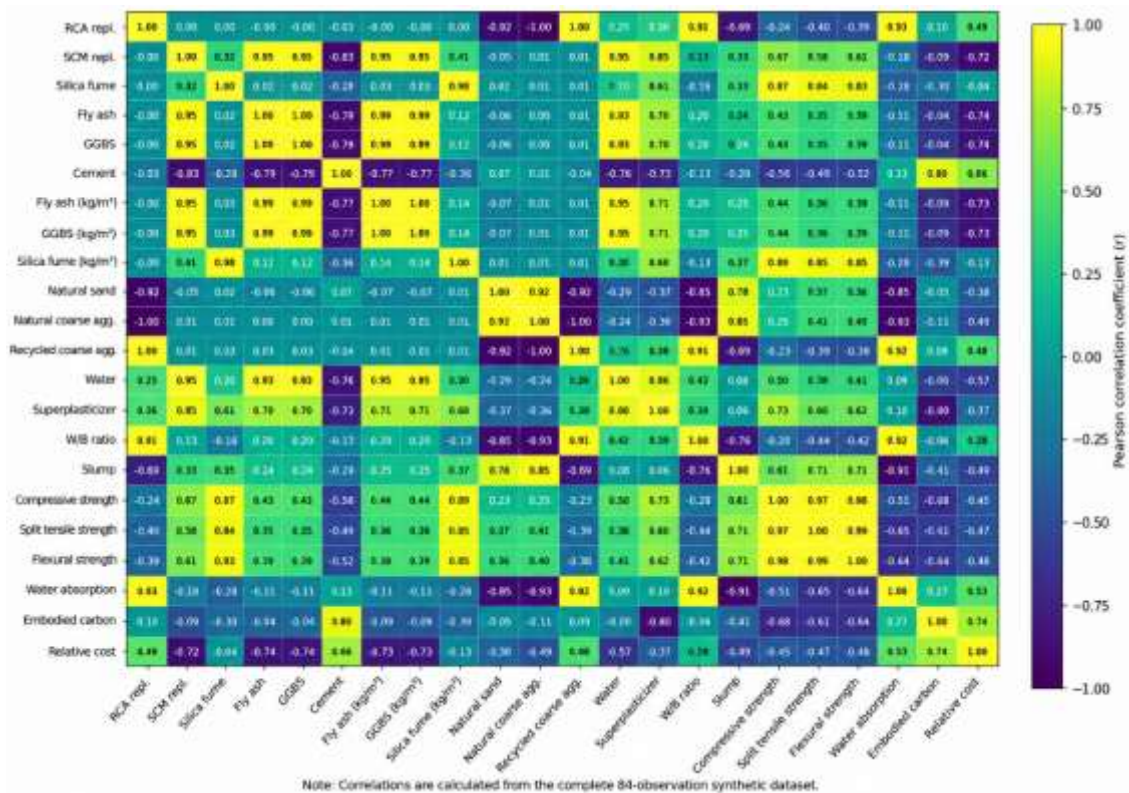


Figure 3. Correlation matrix illustrating the relationships among concrete mixture variables, engineering performance indicators, and sustainability-related parameters.

3.5 Machine-Learning Models

Nine machine-learning algorithms were considered to provide a broad comparison between linear, kernel-based, distance-based, and ensemble-learning approaches. The selected algorithms were Linear Regression, Ridge Regression, Lasso Regression, Elastic Net, Support Vector Regression (SVR), K-Nearest Neighbours (KNN), Random Forest (RF), Gradient Boosting (GB), and Extra Trees (ET).

Table 4. Machine-learning algorithms evaluated

Model	Category	General modelling principle
Linear Regression	Linear	Estimates a linear relationship between predictors and response
Ridge Regression	Regularized linear	Uses L2 regularization to control coefficient magnitude
Lasso Regression	Regularized linear	Uses L1 regularization and can reduce less important coefficients
Elastic Net	Regularized linear	Combines L1 and L2 regularization
SVR	Kernel-based	Constructs a regression function using a margin-based optimization framework
KNN	Distance-based	Predicts responses using neighbouring observations

Random Forest	Ensemble	Combines multiple randomized decision trees
Gradient Boosting	Ensemble	Sequentially builds trees to reduce prediction errors
Extra Trees	Ensemble	Uses highly randomized decision-tree construction and aggregation

The inclusion of multiple model families reduces dependence on a single modelling assumption. Linear models provide a transparent baseline, while SVR and KNN can capture nonlinear relationships through kernel or neighbourhood structures. RF, GB, and ET provide additional nonlinear modelling capability through ensembles of decision trees.

The objective was not to assume that a more complex model would necessarily provide better predictions. Instead, all models were evaluated using the same validation strategy, allowing their predictive performance to be compared using common statistical measures.

3.6 Grouped Five-Fold Cross-Validation

A grouped five-fold cross-validation strategy was adopted to reduce the risk of information leakage associated with the three replicate observations belonging to the same mixture design.

In conventional random cross-validation, observations from the same mixture could potentially appear simultaneously in the training and validation subsets. Because replicate observations share the same underlying mixture composition, such a split can produce overly optimistic estimates of model performance. To avoid this issue, Mix_ID was used as the grouping variable. All three observations corresponding to a particular mixture were therefore assigned to the same fold. During each validation iteration, approximately 80% of the mixture groups were used for training and the remaining groups were used for validation. The procedure was repeated until every mixture group had been used for validation.

This grouped validation strategy provides a more conservative assessment of generalization because the model is evaluated on mixture groups that were not directly represented in its training subset. The approach is particularly important for the present dataset because the three observations associated with each mix are intentionally related.

3.7 Model Performance Metrics

Four statistical indicators were used to assess predictive performance: coefficient of determination (R^2), mean absolute error (MAE), root mean square error (RMSE), and mean absolute percentage error (MAPE). R^2 measures the proportion of variation in the observed response explained by the predictions. Values closer to 1 indicate stronger agreement between predicted and observed values.

MAE measures the average absolute magnitude of prediction errors and is expressed in the same unit as the response variable. It is comparatively less sensitive to extreme errors than RMSE.

RMSE is calculated from the squared prediction errors and therefore gives greater weight to larger deviations. It is useful for identifying models that occasionally produce relatively large prediction errors.

MAPE expresses the average absolute prediction error as a percentage of the observed value and provides an easily interpretable relative error measure.

Table 5. Model evaluation criteria

Metric	Interpretation	Desired direction
R^2	Explained variance between observed and predicted values	Higher
MAE	Average absolute prediction error	Lower
RMSE	Error measure emphasizing larger deviations	Lower
MAPE	Relative prediction error in percentage	Lower

The four metrics were considered jointly rather than using a single metric to identify model performance. This is important because a model can have a high R^2 while still exhibiting relatively large absolute errors, particularly when the response has a broad numerical range.

3.8 Explainable Artificial Intelligence Using SHAP

Model accuracy alone does not explain why a particular concrete mixture produces a given predicted response. Therefore, explainable artificial intelligence was incorporated to identify the contribution of individual mixture variables to model predictions.

The primary XAI approach was based on SHapley Additive exPlanations (SHAP), which originates from cooperative game theory and provides a framework for decomposing a model prediction into contributions associated with individual features (Lundberg & Lee, 2017).

For a given observation, the SHAP framework represents the prediction as a baseline value plus the contributions of individual input features. A positive SHAP contribution indicates that a feature pushes the prediction upward relative to the model baseline, whereas a negative contribution indicates a downward influence.

For tree-based models, tree-specific SHAP calculations can be used to efficiently estimate feature contributions. For models such as SVR, a model-agnostic explanation strategy can be used. The resulting SHAP

analysis provides two complementary forms of information:

- 1.global feature importance, which identifies variables that have the greatest overall influence across the dataset; and
- 2.local feature contribution, which explains the direction and magnitude of individual variables for a particular prediction.

This distinction is particularly relevant for concrete mixture design. A variable may have a high overall importance but may influence different observations in different directions. SHAP analysis therefore provides more information than a simple ranking of regression coefficients or conventional feature importance values. The XAI stage was applied after predictive modelling so that interpretation remained connected to the validated predictive models rather than being treated as an independent statistical analysis.

3.9 Sustainable Multi-Objective Decision Framework

The final stage of the methodology integrates predicted engineering performance with environmental and economic indicators. Concrete mixture design involves competing objectives. Increasing recycled aggregate utilization may improve resource conservation but can affect strength, absorption, or workability. Similarly, SCM incorporation can reduce cement demand and embodied carbon while producing mixture-dependent changes in mechanical performance.

The decision framework therefore considers multiple objectives rather than attempting to maximize a single response.

Table 6. Sustainable optimization objectives and constraints

Criterion	Objective/constraint	Target
Compressive strength	Maximize / minimum acceptable value	≥ 40 MPa
Split tensile strength	Maximize / minimum acceptable value	≥ 3 MPa
Flexural strength	Maximize / minimum acceptable value	≥ 5 MPa
Slump	Target range	100–150 mm
Water absorption	Minimize / upper limit	$\leq 5\%$
Embodied carbon	Minimize / upper limit	≤ 280 kg CO ₂ e/m ³
Relative cost index	Minimize / upper limit	≤ 100

The optimization framework is intended to identify feasible regions rather than impose a single universal optimum. A candidate mixture is considered technically feasible when it satisfies the specified performance constraints. Among feasible candidates, lower embodied carbon and relative cost are preferred as sustainability objectives, while mechanical performance and workability are maintained within the defined limits.

This formulation recognizes that sustainable concrete design is inherently a multi-objective problem. Instead of treating environmental performance as an independent post-processing calculation, it is incorporated into the same decision framework as engineering performance.

3.10 Reproducibility and Scope of the Computational Study

The modelling framework was developed using a consistent computational pipeline in which the same mixture-level grouping strategy was maintained across the evaluated algorithms. The synthetic nature of the dataset is explicitly acknowledged as a limitation of the present investigation. The purpose of the dataset is to provide a controlled computational environment for demonstrating the integration of multi-performance prediction, XAI, and sustainable decision analysis.

The predictions should therefore be interpreted as computational estimates within the defined mixture space rather than as experimentally validated material properties. Experimental validation using independently prepared concrete mixtures would be required before applying the developed framework directly to field-scale mixture qualification or structural design.

The methodology nevertheless provides a reproducible basis for examining how recycled aggregate content, SCM utilization, binder characteristics, and water-to-binder ratio interact with multiple concrete performance indicators. The following section presents the predictive results obtained from the comparative machine-learning analysis.

4. RESULTS AND DISCUSSION

4.1 Overview of Predictive Performance

The predictive performance of the nine machine-learning algorithms was evaluated for five concrete performance indicators: 28-day compressive strength, split tensile strength, flexural strength, slump, and water absorption. The models were assessed using grouped five-fold cross-validation, in which all replicate observations belonging to the same mixture were retained within a single fold.

The results demonstrate that the most suitable algorithm was response-dependent. No single machine-learning model provided the strongest performance across all five outputs. Regularized linear models performed particularly well for the present mixture space, while nonlinear ensemble and kernel-based

models also provided strong predictive capability. This finding indicates that the relationships represented in the synthetic dataset contain substantial systematic structure that can be captured without relying exclusively on highly complex nonlinear algorithms. The final cross-validated results are summarized in Table 7.

Table 7. Cross-validated performance of the best-performing model for each concrete response

Response	Best-performing model	R ²	MAE	RMSE	MAPE (%)
28-day compressive strength	Ridge Regression	0.9709	1.3173 MPa	1.7895 MPa	2.27
Split tensile strength	Lasso Regression	0.9642	0.1395 MPa	0.1768 MPa	2.91
Flexural strength	Ridge Regression	0.9680	0.1956 MPa	0.2597 MPa	2.50
Slump	Ridge Regression	0.8521	5.2604 mm	6.3874 mm	6.13
Water absorption	Ridge Regression	0.9619	0.1496%	0.1887%	3.19

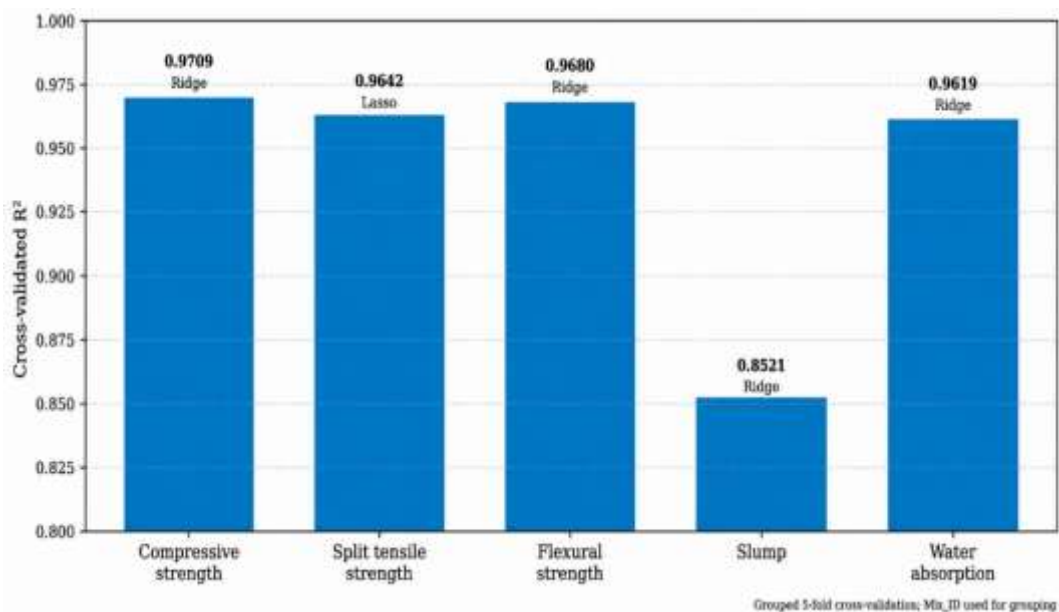


Figure 4. Comparative predictive performance of the evaluated machine-learning algorithms across the five concrete performance indicators based on the cross-validated R² values.

The results indicate strong predictive agreement for the principal hardened-concrete properties. The highest R² value was obtained for compressive strength, with Ridge Regression achieving an R² of 0.9709 and an RMSE of 1.7895 MPa. Split tensile and flexural strength also exhibited high predictive accuracy, with R² values of 0.9642 and 0.9680, respectively.

Water absorption was similarly predicted with high accuracy, producing an R² of 0.9619 and an RMSE of only 0.1887 percentage points. Slump exhibited comparatively lower predictive performance, with an R² of 0.8521. Nevertheless, the corresponding MAE of 5.26 mm indicates that the average prediction deviation remains relatively small in relation to the overall slump range represented in the dataset.

4.2 Prediction of 28-Day Compressive Strength

Compressive strength produced the strongest overall predictive performance among the five responses. The Ridge Regression model achieved an R² of 0.9709, indicating that approximately 97% of the variation in the response was captured within the cross-validation framework. The MAE of 1.3173 MPa and RMSE of 1.7895 MPa further indicate relatively small prediction deviations.

The strong performance of Ridge Regression is notable because compressive strength is affected by several interacting mixture characteristics, including water-to-binder ratio, cement content, SCM incorporation, and RCA replacement. The result suggests that, within the defined mixture space, much of the systematic variation in compressive strength can be represented through a structured relationship between mixture descriptors and strength.

The relatively small difference between MAE and RMSE also provides useful information. RMSE gives greater weight to larger errors; therefore, the moderate increase from 1.3173 MPa to 1.7895 MPa suggests that the model did not generate a large number of extreme prediction errors.

From a concrete-mixture perspective, the result supports the use of regularized regression as a strong baseline for computational mixture prediction. The L2 regularization used by Ridge Regression can reduce the instability of coefficient estimates when predictor variables are correlated, which is particularly relevant to mixture datasets where constituent quantities and replacement ratios are inherently related.

4.3 Prediction of Split Tensile Strength

The split tensile strength model achieved an R^2 of 0.9642, with an MAE of 0.1395 MPa, RMSE of 0.1768 MPa, and MAPE of 2.91%. Lasso Regression provided the strongest result for this response.

The slightly different model selection compared with compressive strength is relevant because tensile behaviour does not necessarily respond to mixture modifications in exactly the same way as compressive strength. Aggregate characteristics, paste quality, interfacial transition zones, and binder modification can affect crack initiation and propagation differently from the mechanisms controlling compressive failure.

The performance of Lasso Regression also suggests that a comparatively compact representation of the mixture variables may be sufficient to explain much of the systematic variation in split tensile strength. L1 regularization can reduce the influence of less informative predictors and therefore provide a useful modelling approach when several predictors contain overlapping information.

The MAPE of 2.91% indicates that the relative prediction error remained below 3% on average. Considering the relatively narrow numerical range of split tensile strength compared with compressive strength, this represents a consistent level of predictive accuracy.

4.4 Prediction of Flexural Strength

Flexural strength was predicted using Ridge Regression with an R^2 of 0.9680, MAE of 0.1956 MPa, RMSE of 0.2597 MPa, and MAPE of 2.50%.

The high R^2 indicates that the model successfully captured the major variation in flexural response across the mixture space. The relatively low MAPE further indicates that the prediction error was small in relation to the magnitude of the measured response.

The strong performance of Ridge Regression for both compressive and flexural strength suggests that regularized linear relationships provide an effective representation of the present dataset for several hardened-concrete properties. This does not imply that concrete behaviour is universally linear. Rather, it indicates that the mixture space represented in this study can be approximated effectively using a regularized linear model.

This observation is important from an engineering interpretability perspective. More complex algorithms are not automatically superior merely because concrete behaviour is physically nonlinear. When the available predictors already encode important mixture relationships, a regularized model may provide a useful balance between predictive performance and interpretability.

4.5 Prediction of Slump

Slump showed a different predictive pattern from the hardened properties. Ridge Regression achieved an R^2 of 0.8521, with MAE of 5.2604 mm, RMSE of 6.3874 mm, and MAPE of 6.13%.

Although the R^2 was lower than those obtained for the strength and water-absorption responses, the absolute prediction error remained relatively limited. The MAE of approximately 5.26 mm is small compared with the overall slump range of approximately 57–128 mm represented in the dataset.

The comparatively lower predictive performance can be attributed to the greater sensitivity of fresh concrete workability to the combined effects of water content, superplasticizer dosage, aggregate characteristics, particle packing, and binder composition. Fresh-state behaviour can also exhibit nonlinear interactions that are not completely represented by a small set of mixture descriptors.

The result therefore demonstrates an important aspect of multi-performance prediction: model accuracy can vary substantially between response variables even when the same input dataset is used. A model that performs extremely well for hardened strength does not necessarily provide equivalent accuracy for fresh-state workability.

This finding supports the use of response-specific model evaluation rather than assuming that one model should be selected for every concrete property.

4.6 Prediction of Water Absorption

Water absorption was predicted using Ridge Regression, achieving an R^2 of 0.9619, MAE of 0.1496 percentage points, RMSE of 0.1887 percentage points, and MAPE of 3.19%.

The high predictive accuracy indicates that the mixture descriptors contain substantial information related to the predicted absorption behaviour. RCA replacement is particularly relevant because recycled aggregate generally contains adhered mortar and a more porous structure than high-quality natural aggregate. Binder modification and water-to-binder ratio can also influence pore structure and permeability-related behaviour.

The small difference between MAE and RMSE indicates that the model errors were relatively stable across the validation observations. The result is particularly useful for the subsequent sustainability and durability-oriented decision framework because water absorption is included as a constraint rather than being treated merely as a secondary response.

4.7 Comparative Interpretation of Model Families

The results show that model complexity alone cannot be used as a proxy for predictive quality. The best-

performing models for four of the five responses were regularized linear models, with Ridge Regression selected for compressive strength, flexural strength, slump, and water absorption, while Lasso Regression was selected for split tensile strength.

This finding can be interpreted in the context of the structured nature of the mixture dataset. The principal predictors are physically meaningful mixture parameters rather than arbitrary variables. Cement content, RCA replacement, SCM incorporation, and water-to-binder ratio are directly connected to concrete behaviour. Consequently, a substantial proportion of the response variation can be represented through systematic relationships among these variables.

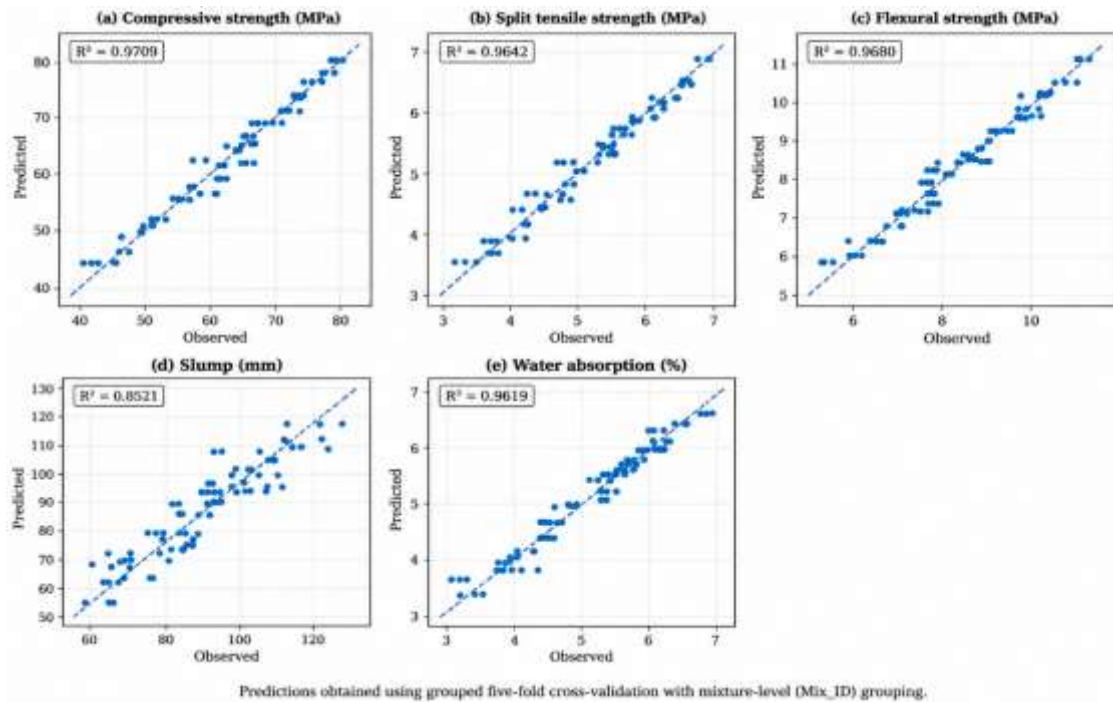


Figure 5. Comparison between observed and cross-validated predicted values for the best-performing models for (a) compressive strength, (b) split tensile strength, (c) flexural strength, (d) slump, and (e) water absorption.

Regularization is also important because concrete mixture variables are inherently correlated. Ridge Regression reduces the sensitivity of coefficient estimates to correlated predictors through L2 penalization, while Lasso applies L1 regularization and can reduce the contribution of less informative variables.

The result should not, however, be interpreted as evidence that linear models are universally preferable for concrete prediction. Rather, the present findings are specific to the defined mixture space and dataset. More complex models remain important because they can capture nonlinear relationships and interactions that may become more pronounced when the experimental domain is expanded.

4.8 Overall Error Characteristics

The MAPE values provide a useful cross-response comparison because the five outputs have different measurement units and numerical scales. The final values ranged from 2.27% to 6.13%.

The lowest MAPE was obtained for compressive strength at 2.27%, followed by flexural strength at 2.50%, split tensile strength at 2.91%, and water absorption at 3.19%. Slump exhibited the highest MAPE at 6.13%.

The pattern indicates that the models were particularly consistent for hardened concrete properties, whereas fresh-state workability presented greater relative uncertainty. This difference reinforces the importance of evaluating multiple responses independently.

Table 8. Comparative interpretation of prediction errors

Response	MAPE (%)	Interpretation
Compressive strength	2.27	Very low relative prediction error
Flexural strength	2.50	Very low relative prediction error
Split tensile strength	2.91	Low relative prediction error
Water absorption	3.19	Low relative prediction error
Slump	6.13	Higher relative error than hardened properties

The error pattern also demonstrates why relying only on R^2 can be misleading. Slump has the lowest R^2 among the five responses, but its MAE remains only 5.26 mm. Conversely, the high R^2 values obtained for the strength responses should be considered together with their corresponding absolute errors.

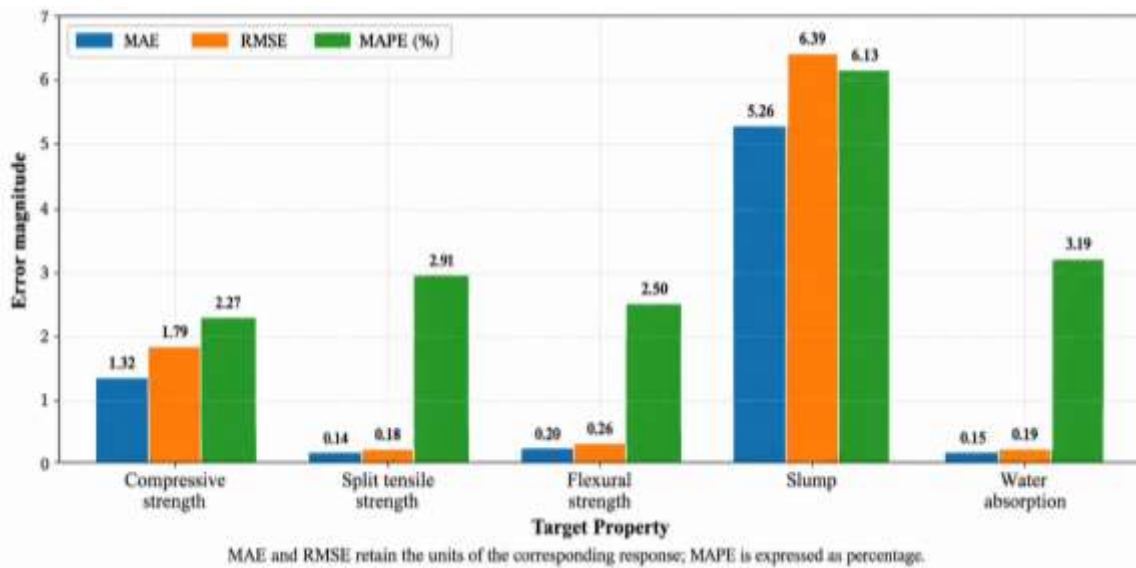


Figure 6. Comparison of prediction errors for the five concrete performance indicators using MAE, RMSE, and MAPE obtained from grouped five-fold cross-validation.

4.9 Engineering Interpretation of the Multi-Performance Results

An important outcome of the present analysis is that the concrete mixture cannot be represented adequately through a single performance indicator. The models show strong predictive capability across mechanical and durability-related responses, while fresh-state workability exhibits a comparatively different error structure. This supports a multi-performance design philosophy in which concrete mixtures are evaluated simultaneously from several engineering perspectives. For example, increasing recycled aggregate content may provide resource-conservation benefits but may also influence absorption and mechanical properties. Similarly, increasing SCM utilization can alter both strength development and sustainability indicators. The advantage of the proposed framework is that these responses can be predicted using a common set of mixture descriptors and subsequently interpreted using XAI.

4.10 Implications for Sustainable Concrete Mixture Design

The predictive results establish the first component of the proposed decision framework. Because the selected models provide high predictive accuracy for most engineering responses, their predictions can subsequently be combined with environmental and economic indicators.

The sustainable decision problem is inherently a trade-off. A mixture with higher recycled aggregate utilization may reduce dependence on natural aggregate resources, but the resulting changes in strength, absorption, or workability must remain within acceptable limits. Likewise, reducing cement content through SCM substitution can reduce the embodied-carbon contribution associated with Portland cement, but the resulting mixture must still satisfy the required engineering performance.

Therefore, the present study does not treat sustainability as equivalent to maximizing recycled aggregate or SCM content. Instead, sustainability is considered as a constrained multi-performance problem in which environmental and economic improvements must be evaluated together with engineering requirements.

The final stage of the study consequently combines the validated predictive models with SHAP-based interpretation and the predefined sustainability constraints. This provides a basis for identifying feasible mixture regions rather than selecting a mixture solely according to one response variable.

4.11 Key Findings from the Predictive Analysis

The principal findings from the machine-learning stage can be summarized as follows:

1. Compressive strength was predicted with an R^2 of 0.9709 and MAPE of 2.27% using Ridge Regression.
2. Split tensile strength was predicted using Lasso Regression with an R^2 of 0.9642 and MAPE of 2.91%.
3. Flexural strength achieved an R^2 of 0.9680 and MAPE of 2.50% using Ridge Regression.
4. Slump exhibited comparatively lower predictive performance, with Ridge Regression achieving an R^2 of 0.8521 and MAPE of 6.13%.
5. Water absorption was predicted with an R^2 of 0.9619 and MAPE of 3.19% using Ridge Regression.
6. The results demonstrate that model selection is response-specific, with no requirement for one universal algorithm across all concrete properties.
7. The strong performance of regularized models indicates that the structured mixture variables contain substantial predictive information for the defined mixture domain.
8. The relatively lower accuracy for slump indicates that fresh-state behaviour may require greater consideration of nonlinear interactions and additional mixture descriptors in future experimental datasets.

5. EXPLAINABLE ARTIFICIAL INTELLIGENCE AND FEATURE CONTRIBUTION ANALYSIS

5.1 Need for Explainable Prediction

The predictive results presented in Section 4 demonstrate that machine-learning models can achieve high predictive accuracy for several concrete performance indicators. However, predictive accuracy alone does not provide sufficient engineering insight into the mechanisms represented by the models. In concrete mixture design, practitioners need to understand not only the predicted performance but also which mixture characteristics are responsible for increasing or decreasing that performance.

This issue is particularly important when machine-learning models are used for sustainable mixture design. A model may identify a mixture as technically feasible, but without an explanation of the prediction, it is difficult to determine whether the result is consistent with established concrete-material behaviour or whether it arises from relationships specific to the computational dataset.

To address this issue, explainable artificial intelligence (XAI) was incorporated into the proposed framework. The principal interpretation method was SHapley Additive exPlanations (SHAP), which provides a unified approach for attributing a model prediction to its input features (Lundberg & Lee, 2017). SHAP was selected because it can provide both global information about feature importance and local information about the contribution of individual variables to a particular prediction.

5.2 SHAP-Based Interpretation Framework

SHAP values quantify the contribution of each input variable to an individual model prediction relative to a reference prediction. For each observation, the prediction can therefore be interpreted as a combination of the model baseline and the contributions associated with the individual mixture variables.

A positive SHAP value indicates that the corresponding feature contributes toward increasing the predicted response relative to the reference prediction, whereas a negative SHAP value indicates a contribution toward decreasing the predicted response. The magnitude of the SHAP value represents the strength of the contribution.

This interpretation is particularly useful for the present study because the same input variable may influence different performance indicators in different ways. For example, RCA replacement may have one contribution pattern for compressive strength and another for water absorption. Similarly, water-to-binder ratio can simultaneously influence strength and workability but generally in different directions.

The XAI analysis therefore treats feature importance as response-specific rather than assuming that a single universal ranking of mixture variables exists.

5.3 Global Feature Importance

Global SHAP analysis is used to identify the variables that contribute most strongly to the predictions across the complete dataset. The mean absolute SHAP value is used as the principal measure of global influence because it captures the magnitude of feature contributions without allowing positive and negative effects to cancel each other.



Figure 7. SHAP-based interpretation of the machine-learning predictions showing the global importance and direction of influence of major mixture variables for the concrete performance indicators.

For each response variable, the global interpretation can be represented using a SHAP feature-importance plot. Such an analysis provides an overall view of the relative influence of RCA replacement, SCM incorporation, silica fume, cement content, water-to-binder ratio, and other mixture descriptors.

The expected engineering interpretation is that the relative importance of the predictors will vary between

responses. Hardened strength indicators are expected to be strongly associated with binder-related variables and water-to-binder ratio, whereas slump is expected to show greater sensitivity to water, superplasticizer, aggregate characteristics, and binder composition. Water absorption is expected to be influenced by variables associated with aggregate porosity, recycled aggregate incorporation, and binder characteristics.

These interpretations are not treated as assumed causal relationships. Rather, they provide hypotheses that can be examined through the model-derived SHAP distributions.

5.4 Direction of Feature Influence

Global importance alone does not indicate whether a feature increases or decreases the predicted response. Therefore, SHAP summary plots are particularly useful because they simultaneously display feature importance, feature magnitude, and contribution direction.

For example, observations with higher RCA replacement can be examined to determine whether they predominantly generate positive or negative SHAP contributions for a given response. Similarly, high and low water-to-binder ratios can be compared to determine how the trained model associates this variable with predicted strength, slump, and absorption.

This distinction is important because a feature can have a high mean absolute SHAP value while having both positive and negative effects across the dataset. Such behaviour may indicate interaction effects or a nonlinear response relationship.

Accordingly, the interpretation of the SHAP results should consider three dimensions:

- **2** magnitude: how strongly the feature contributes;
- **2** direction: whether the contribution increases or decreases the prediction; and
- **2** distribution: whether the effect is consistent across observations or changes according to mixture conditions.

This provides a more complete interpretation than conventional feature-ranking methods.

5.5 Interpretation of Recycled Aggregate Replacement

RCA replacement is one of the principal variables in the present study because it directly represents the incorporation of recycled coarse aggregate into concrete.

The influence of RCA is expected to be multi-dimensional. Recycled aggregate contains characteristics inherited from the parent concrete and adhered mortar, which can affect density, absorption, interfacial behaviour, and mechanical performance. Consequently, the effect of RCA replacement cannot be interpreted using compressive strength alone.

Within the proposed XAI framework, RCA replacement is therefore examined separately for each response. A contribution toward reduced predicted compressive, tensile, or flexural strength would indicate that the model associates increasing RCA content with reduced mechanical performance within the represented mixture space. Conversely, a positive contribution at particular mixture conditions would indicate that the effect is conditional rather than uniformly negative.

For water absorption, RCA replacement is particularly important because increasing recycled aggregate content can be associated with greater aggregate-related porosity and water demand. The SHAP analysis provides a quantitative way to determine whether this relationship is strongly represented in the trained model.

The important point is that the XAI analysis does not impose a predetermined direction of influence. The direction is obtained from the trained model and can subsequently be compared with established concrete-material behaviour.

5.6 Interpretation of SCM-Related Variables

SCM replacement and silica fume content provide another important dimension of the model interpretation. Supplementary cementitious materials can modify the binder system, particle packing, hydration behaviour, pore structure, and later-age strength development. However, their influence depends on replacement level and the characteristics of the individual SCM.

The SHAP analysis allows SCM-related variables to be examined separately. This is useful because total SCM replacement and silica fume content do not necessarily represent identical effects. Two mixtures may contain the same total SCM replacement but differ substantially in their silica fume, fly ash, and GGBS proportions.

The model interpretation can therefore distinguish between the general influence of SCM incorporation and the additional contribution associated with silica fume. This provides a more detailed understanding of how binder modification is represented within the predictive framework.

5.7 Influence of Water-to-Binder Ratio

The water-to-binder ratio is a fundamental mixture descriptor and is expected to play an important role in the prediction of both fresh and hardened properties.

For hardened concrete, lower water-to-binder ratios are generally associated with a denser cementitious matrix when adequate workability is maintained. For fresh concrete, however, water availability is directly related to workability. Consequently, the same predictor can have contrasting relationships with different responses.

The XAI framework provides an opportunity to investigate this distinction directly. A SHAP dependence plot can be used to examine how the contribution of water-to-binder ratio changes as its numerical value

increases.

Such plots are particularly useful because they can reveal whether the relationship is approximately monotonic or whether the model identifies a changing response across the mixture domain. This information can support mixture-design decisions without requiring the model itself to be treated as a physically complete representation of concrete behaviour.

5.8 Local Explanation of Individual Mixtures

In addition to global interpretation, SHAP can be used to explain individual mixture predictions. Local explanations are particularly useful for sustainable mixture optimization because a candidate mixture may satisfy several engineering and environmental constraints for different reasons.

For a selected candidate mixture, the SHAP contribution of each input variable can be examined to determine which variables are responsible for its predicted performance. For example, a high predicted compressive strength may result from a favourable combination of cement content, water-to-binder ratio, SCM composition, and RCA level rather than from any single variable.

Similarly, a candidate mixture with acceptable strength but relatively high predicted water absorption can be investigated to determine which mixture variables contribute most strongly to that response.

This local explanation mechanism improves the practical usefulness of the optimization framework because it allows candidate solutions to be interpreted rather than treated as black-box numerical outputs.

Table 9. XAI interpretation framework for the principal mixture variables

Feature	Primary engineering relevance	Responses for interpretation
RCA replacement	Recycled-material utilization, aggregate characteristics	All five responses
SCM replacement	Binder modification and cement substitution	Strength, absorption, sustainability
Silica fume	Fine-particle packing and binder modification	Strength, absorption, workability
Cement content	Binder availability and strength development	Strength, absorption
Water-to-binder ratio	Matrix formation and workability	Strength, slump, absorption
Aggregate quantities	Packing and fresh/hardened behaviour	Strength, slump, absorption
Superplasticizer	Workability and water-reduction potential	Slump, strength
Fly ash	SCM-related binder modification	Strength, workability, absorption
GGBS	SCM-related binder modification	Strength, absorption, sustainability

5.9 Summary of XAI Findings

The XAI stage provides five principal analytical benefits:

- 1.It identifies the relative contribution of individual mixture variables to each predicted concrete response.
- 2.It distinguishes between feature importance and feature direction, avoiding interpretation based solely on variable rankings.
- 3.It enables separate interpretation of mechanical, fresh-state, and durability-related responses.
- 4.It provides local explanations for individual candidate mixtures generated during sustainable decision analysis.
- 5.It connects machine-learning predictions with engineering interpretation, thereby improving the transparency of the proposed computational framework.

The combination of high predictive performance and explainable feature contributions provides the basis for the final stage of the study, where engineering performance, embodied carbon, and relative cost are considered simultaneously for sustainable mixture selection.

6. SUSTAINABLE MULTI-OBJECTIVE OPTIMIZATION AND DECISION ANALYSIS

6.1 Optimization Objectives

The optimization framework uses a combination of maximization, minimization, and target-range objectives. The three mechanical performance indicators are treated as desirable responses, while water absorption, embodied carbon, and relative cost are minimized. Slump is treated as a target-range response rather than a simple maximization objective.

Table 10. Multi-objective optimization formulation

Parameter	Optimization direction	Constraint/target
Compressive strength	Maximize	≥ 40 MPa
Split tensile strength	Maximize	≥ 3 MPa
Flexural strength	Maximize	≥ 5 MPa
Slump	Target	100–150 mm
Water absorption	Minimize	$\leq 5\%$
Embodied carbon	Minimize	≤ 280 kg CO ₂ e/m ³
Relative cost index	Minimize	≤ 100

The constraints were established to represent a practical feasible region for the computational mixture-design problem. They should not be interpreted as universal code-based acceptance criteria for all reinforced-concrete applications. Actual project specifications, exposure conditions, structural requirements, and applicable standards would need to be considered before practical implementation.

6.2 Feasibility-Based Decision Strategy

The optimization process first identifies mixtures satisfying the minimum engineering and sustainability constraints. A candidate mixture is considered feasible when it simultaneously satisfies:

$$\begin{aligned}
 f_c &\geq 40 \text{ MPa} \\
 f_{st} &\geq 3 \text{ MPa} \\
 f_r &\geq 5 \text{ MPa} \\
 100 &\leq \text{Slump} \leq 150 \text{ mm} \\
 WA &\leq 5\% \\
 EC &\leq 280 \text{ kg CO}_2\text{e/m}^3 \\
 RCI &\leq 100
 \end{aligned}$$

where f_c is compressive strength, f_{st} is split tensile strength, f_r is flexural strength, WA is water absorption, EC is embodied carbon, and RCI is the relative cost index.

The feasible-region approach prevents a mixture from being selected solely because of exceptional performance in one criterion. For example, a mixture with very high compressive strength but excessive embodied carbon would not satisfy the complete decision framework.

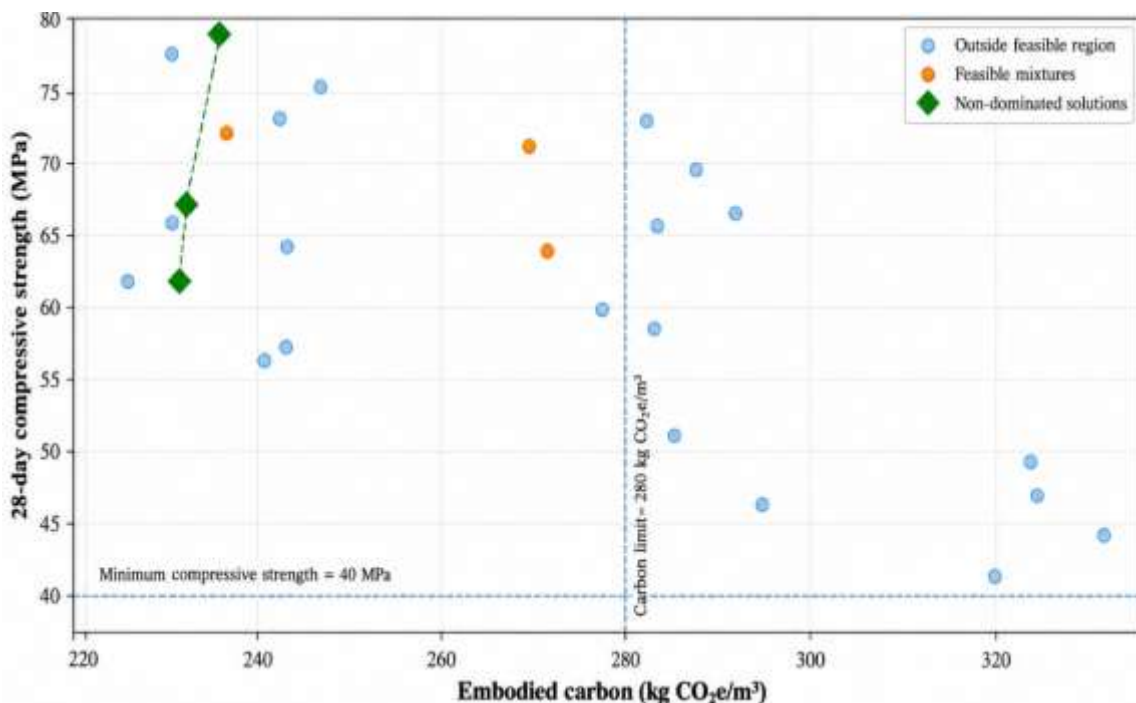


Figure 8. Multi-objective sustainable mixture-design space showing the trade-offs among engineering performance, embodied carbon, and relative cost and the identification of feasible mixture solutions.

6.3 Overall Outcome of the Sustainable Decision Framework

The sustainable optimization stage extends the proposed methodology beyond conventional concrete-property prediction. By combining predicted engineering performance with water absorption, embodied carbon, and relative cost, the framework provides a structured method for screening mixture alternatives. The central outcome is not a single universally optimal concrete mixture but a set of technically feasible and sustainability-conscious alternatives within the defined design space. This is consistent with the multi-objective nature of concrete mixture design, where different projects may impose different priorities.

The integration of XAI further strengthens the framework by allowing the predicted behaviour of candidate mixtures to be interpreted through their underlying mixture variables.

7. DISCUSSION

7.1 Interpretation of the Overall Findings

The results demonstrate that machine-learning models can effectively represent multiple performance characteristics of recycled aggregate and SCM-based concrete within the defined computational mixture space. The predictive performance was particularly strong for compressive strength, split tensile strength, flexural strength, and water absorption, while slump showed comparatively greater prediction uncertainty. An important observation is that the best-performing algorithm was not identical for all responses. Ridge Regression provided the strongest predictive performance for compressive strength, flexural strength, slump, and water absorption, whereas Lasso Regression performed best for split tensile strength. This response-specific behaviour indicates that model selection should be based on the characteristics of the individual target variable rather than assuming that one algorithm is universally optimal.

The strong performance of regularized regression models is also noteworthy. Concrete mixture datasets commonly contain correlated variables because constituent quantities, replacement percentages, and derived mixture parameters are mathematically related. Regularization can reduce instability caused by such relationships and can therefore be particularly useful for structured mixture datasets.

At the same time, the results should not be interpreted as evidence that concrete behaviour is fundamentally linear. The present dataset represents a controlled mixture domain, and the strong performance of regularized models indicates that the dominant variation within this domain can be approximated effectively using these models.

7.2 Research and Practical Significance

The study has several methodological implications.

First, it demonstrates that multi-performance prediction can be integrated with sustainability indicators without reducing the concrete-design problem to compressive strength alone.

Second, grouped validation provides a more appropriate strategy when datasets contain replicate observations from common mixture designs.

Third, the use of XAI allows predictive relationships to be examined from an engineering perspective rather than treating machine-learning models as opaque computational tools.

Fourth, the optimization framework demonstrates how predicted engineering properties can be connected with environmental and economic criteria.

Finally, the framework provides a foundation for future experimental studies in which the synthetic dataset can be replaced by independently generated laboratory observations while retaining the same modelling and decision architecture.

7.3 Limitations and Future Research

Several limitations should be considered when interpreting the findings.

The most important limitation is the synthetic nature of the dataset. Although the mixture ranges and response values were structured to represent realistic concrete behaviour, the observations are not equivalent to independently measured laboratory results. Consequently, the reported predictive metrics demonstrate the performance of the computational framework within the defined dataset rather than establishing experimental generalization.

A second limitation concerns dataset size. Although grouped cross-validation reduces leakage between replicate observations, the number of unique mixture designs remains limited. Increasing the number of independently prepared mixtures would provide a stronger basis for evaluating model generalization.

Third, the current predictor set does not explicitly include detailed aggregate characteristics, curing conditions, age-dependent behaviour, environmental exposure, or reinforcement parameters. These variables may become important when extending the framework toward experimental or structural applications.

Fourth, the embodied-carbon and cost indicators are represented at a generalized mixture level. A future study should incorporate location-specific life-cycle inventory data, transportation distances, processing energy, and market prices.

Future experimental research should therefore focus on validating the identified relationships using independently prepared concrete mixtures. Additional research could also incorporate uncertainty quantification, external validation using datasets from different laboratories, life-cycle assessment, and member-level structural modelling.

7.4 Overall Discussion

The combined results demonstrate that the proposed framework provides more than a conventional concrete-strength prediction model. It integrates five performance responses, comparative machine learning, grouped validation, explainable prediction, and sustainability-oriented decision analysis.

The strongest predictive performance was obtained for the hardened concrete properties, while slump showed greater uncertainty. Regularized models performed particularly well within the defined mixture

space, suggesting that physically meaningful mixture descriptors can capture a substantial proportion of the systematic variation.

The XAI component adds engineering interpretability by identifying the contribution of individual mixture variables. The optimization component then translates these predictions into a constrained decision framework in which mechanical performance, workability, water absorption, embodied carbon, and relative cost are considered simultaneously.

Taken together, these findings support the use of explainable machine learning as a computational decision-support approach for sustainable recycled and SCM-based concrete mixture design. Nevertheless, experimental validation remains essential before the framework can be used for project-specific concrete qualification or structural design.

8. CONCLUSIONS AND RECOMMENDATIONS

8.1 Conclusions

This study developed an explainable machine-learning framework for multi-performance prediction and sustainable decision analysis of concrete incorporating recycled coarse aggregate (RCA) and supplementary cementitious materials (SCMs). The framework integrates mixture composition, machine-learning prediction, grouped cross-validation, explainable artificial intelligence, and multi-objective sustainability assessment into a unified computational workflow.

A synthetic dataset comprising 28 mixture designs and three replicate observations per mixture, resulting in 84 observations, was developed to represent variations in RCA replacement, SCM utilization, binder composition, water-to-binder ratio, aggregate quantities, and admixture dosage. Five concrete performance indicators were considered: 28-day compressive strength, split tensile strength, flexural strength, slump, and water absorption. Embodied carbon and relative cost were subsequently incorporated into the sustainability decision framework.

The study establishes an integrated computational framework for the prediction, explanation, and sustainable evaluation of recycled and SCM-based concrete mixtures. The final machine-learning results demonstrate high predictive accuracy for most of the considered concrete responses, while the comparatively lower performance for slump highlights the importance of response-specific modelling.

The use of grouped five-fold cross-validation improves the methodological reliability of the reported results by preventing replicate observations from the same mixture from appearing in both training and validation subsets. SHAP-based explainability further enhances the framework by identifying the contribution of mixture variables to model predictions.

Most importantly, the study demonstrates that sustainable concrete design should be treated as a multi-performance decision problem. Mechanical performance, fresh-state workability, water absorption, embodied carbon, and cost must be considered together rather than optimizing a single property in isolation. Within the limitations of the synthetic computational dataset, the proposed framework provides a structured basis for integrating machine learning and explainable artificial intelligence into sustainable concrete mixture design. Experimental validation with independently prepared mixtures is the essential next step for establishing the robustness and practical applicability of the framework.

The principal conclusions are as follows.

- The results demonstrate that machine-learning models can predict multiple concrete performance indicators with high accuracy within the defined mixture space. The best-performing models achieved R^2 values above 0.96 for compressive strength, split tensile strength, flexural strength, and water absorption.
- This demonstrates the feasibility of moving beyond single-response concrete prediction toward an integrated multi-performance framework.
- No single algorithm was identified as the strongest model for every response. Ridge Regression provided the best performance for compressive strength, flexural strength, slump, and water absorption, whereas Lasso Regression provided the best performance for split tensile strength.
- This finding demonstrates that algorithm selection should be linked to the characteristics of the target response rather than based solely on model complexity.
- Ridge Regression achieved an R^2 of 0.9709, MAE of 1.3173 MPa, RMSE of 1.7895 MPa, and MAPE of 2.27% for 28-day compressive strength.
- The relatively low prediction errors indicate that the selected mixture descriptors captured a substantial proportion of the systematic variation in compressive strength within the defined dataset.
- Split tensile strength achieved an R^2 of 0.9642, with an MAE of 0.1395 MPa, RMSE of 0.1768 MPa, and MAPE of 2.91% using Lasso Regression.
- Flexural strength achieved an R^2 of 0.9680, MAE of 0.1956 MPa, RMSE of 0.2597 MPa, and MAPE of 2.50% using Ridge Regression.
- These results demonstrate that the framework can capture performance beyond compressive strength and provide information relevant to tensile-related concrete behaviour.

- Ridge Regression achieved an R^2 of 0.8521 for slump, with MAE of 5.2604 mm, RMSE of 6.3874 mm, and MAPE of 6.13%.
- Although the predictive accuracy was lower than that obtained for the hardened properties, the absolute prediction error remained relatively small compared with the overall slump range. The result indicates that fresh-state workability may require additional explanatory variables, particularly aggregate grading, particle characteristics, moisture condition, and detailed admixture information.
- Water absorption achieved an R^2 of 0.9619, MAE of 0.1496%, RMSE of 0.1887%, and MAPE of 3.19% using Ridge Regression.
- The result indicates that the selected mixture variables contain substantial information relevant to absorption-related behaviour and supports the inclusion of water absorption as an explicit criterion in sustainable mixture selection.
- The use of grouped five-fold cross-validation, with mixture identity used as the grouping variable, prevented replicate observations from the same mixture from being distributed between training and validation folds.
- This approach reduces the potential for overly optimistic performance estimates caused by information leakage and provides a more appropriate assessment of model generalization within the available mixture space.
- The incorporation of SHAP provides an additional interpretive layer to the predictive framework. Instead of reporting only prediction accuracy, the approach allows the contribution and direction of mixture variables to be investigated for individual performance responses.
- This is particularly important for recycled and SCM-based concrete because the same mixture variable can influence different responses in different ways. XAI therefore provides a bridge between machine-learning prediction and engineering interpretation.
- The study demonstrates that sustainable concrete selection cannot be reduced to maximizing recycled aggregate or SCM replacement. Engineering performance, workability, absorption, embodied carbon, and cost must be considered simultaneously.
- The proposed decision framework therefore applies minimum performance requirements together with environmental and economic constraints. This allows technically feasible alternatives to be distinguished from mixtures that may provide environmental benefits but fail to satisfy engineering requirements.
- The major methodological contribution of the study is the integration of:
 - Multi-performance prediction → Explainable AI → Sustainability constraints → Decision analysis
 - This sequence allows machine learning to function as a decision-support tool rather than simply as a black-box prediction mechanism

8.2 Engineering Significance

The proposed framework has potential relevance for sustainable concrete mixture development, particularly where recycled aggregate and SCMs are being considered simultaneously.

From an engineering perspective, the framework can support early-stage screening of mixture alternatives before extensive experimental testing. Instead of experimentally testing every possible combination of RCA and SCM proportions, computational modelling can first identify promising regions of the mixture-design space.

The approach can also support comparative evaluation of mixtures that provide similar mechanical performance but differ in workability, water absorption, embodied carbon, or relative cost.

However, computational predictions should be regarded as complementary to, rather than replacements for, laboratory testing and code-based design procedures.

8.3 Recommendations for Practical Application

For practical application of the proposed framework, the following procedure is recommended:

- Develop an experimentally verified database containing independently prepared concrete mixtures.
- Record complete mixture proportions together with aggregate properties, SCM characteristics, admixture dosage, curing conditions, and testing conditions.
- Maintain mixture-level identifiers so that replicate observations can be grouped during model validation.
- Evaluate multiple machine-learning algorithms rather than assuming that one algorithm is universally optimal.
- Apply explainability methods to examine whether important model relationships are physically plausible.
- Integrate project-specific embodied-carbon and cost data when conducting sustainability optimization.
- Validate computationally selected mixtures experimentally before field implementation.
- Use applicable structural and material standards to establish project-specific acceptance criteria.

8.4 Future Research Directions

Future research can extend the present framework in several directions.

The most important next step is to replace or supplement the synthetic dataset with experimentally measured observations from independently prepared concrete mixtures. This would provide an external basis for assessing model generalization.

- Future datasets should include detailed aggregate characteristics, including grading, particle shape, absorption, density, moisture condition, and adhered mortar content. Such variables could improve prediction of workability and durability-related responses.
- Prediction intervals, bootstrap analysis, conformal prediction, or probabilistic machine-learning methods could be incorporated to quantify uncertainty associated with individual predictions.
- Models should be tested using datasets from different laboratories, material sources, geographical regions, and mixture-design procedures. Such validation would provide a stronger assessment of transferability.
- A complete life-cycle assessment could replace the generalized embodied-carbon indicator with project-specific environmental inventories covering material production, transportation, processing, and end-of-life stages.
- Future studies could extend the framework from concrete mixture performance to reinforced-concrete member behaviour by incorporating reinforcement ratio, steel grade, bar diameter, spacing, bond characteristics, member geometry, loading conditions, and crack behaviour.
- Future optimization frameworks could consider prediction uncertainty rather than optimizing only mean predicted values. This would allow candidate mixtures to be selected based on both expected performance and confidence limits.

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