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Data-driven prediction and low-carbon optimization of limestone calcined clay cement compressive strength using CPO-XGBoost

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Abstract Limestone calcined clay cement (LC³) is recognized as a promising low-carbon binder owing to its high clinker substitution potential and low-temperature calcination. However, its mix design is hindered by complex nonlinear interactions among multiple components and curing conditions, which traditional empirical models cannot accurately capture. To address this, we develop a CPO-XGBoost model that integrates a crested porcupine optimizer (CPO) with extreme gradient boosting to predict compressive strength. The CPO dynamically balances global exploration and local exploitation, effectively avoiding local optima during hyperparameter tuning. The model achieves excellent predictive accuracy (test $R^2 = 0.938$), outperforming several benchmark algorithms. SHAP and partial dependence plot analyses quantify the marginal effects of each ingredient, identifying optimal composition ranges: clinker 40–55%, calcined clay 25–35%, limestone 15–25%, and gypsum 3–5%. Carbon emission assessment shows a reduction of 41.9–53.2% compared with ordinary Portland cement. An intelligent design system based on Python and Streamlit is also developed for real-time strength prediction and mix optimization, facilitating practical adoption. This work provides a robust data-driven pathway for low-carbon cement production, supporting sustainable construction.

Keywords: Limestone Calcined Clay Cement (LC³); Machine learning; Compressive strength; Carbon reduction; Mix proportion optimization; Sustainable construction materials

1. Introduction

According to the latest report from the International Energy Agency (IEA), the cement industry contributes to approximately 8% of global CO₂ emissions (Dunant et al. 2024). The urgent need for emission reduction has been identified as a core issue in the Global Cement and Concrete Association's (GCCA) 2050 Carbon Neutrality Roadmap. Against this backdrop, the carbon emissions from the cement clinker calcination process have become a shared focus for both the global academic and industrial communities (Elmqvist et al. 2019; Liu et al. 2013). As one of the most promising solutions, limestone calcined clay cement (LC³) is internationally recognized as a low-carbon cement technology with high potential for industrial application, owing to its significant clinker substitution potential (up to 50%) and low-temperature calcination characteristics (approximately 700–900°C) (Avet and Scrivener 2018; Huang et al. 2021; Shao and Cao 2024).

However, the performance control of LC³ concrete faces significant challenges. Compared with traditional Portland cement, the strength development of LC³ is influenced by multi-factor nonlinear coupling, including the reactivity of calcined clay, limestone particle size, gypsum content, curing age, and the synergistic effects of chemical reactions among components (Husain and Jomaa'h 2025; Mukherjee et al. 2025; Shao et al. 2025). This complexity leads to certain performance shortcomings of LC³ in practical applications. Lin et al. (Lin et al. 2022) pointed out that LC³ concrete suffers from issues such as low early-age strength and inadequate carbonation resistance. Further studies by Popa et al. (Popa et al. 2025) demonstrated that while fiber reinforcement can improve its toughness, the strengthening effect varies significantly under different mix proportions. Therefore, the performance of the LC³ system is not governed by a single factor but is the complex outcome of multi-component interactions.

The limitations of traditional strength prediction methods are increasingly evident when addressing this complex system. For a long time, researchers have relied on empirical models such as the Feret equation or Abrams' water-cement ratio law to establish empirical relationships between mix proportions and strength. However, these models are fundamentally based on linear assumptions or simple nonlinear fitting, making it difficult to accurately capture the complex nonlinear interactions within the calcined clay-limestone-clinker system. A systematic review by Li et al. (Li et al. 2022) further pointed out that as the number of components increases and interactions become stronger, the prediction bias of empirical

formulas tends to amplify significantly. Therefore, for a multi-component, highly interactive cementitious system such as LC³, traditional empirical models are no longer sufficient to meet the demands of precise design.

Machine learning has advanced LC³ research, but existing studies suffer from three key limitations: (1) Most models prioritize prediction accuracy over physical interpretability, creating a black box that engineers distrust for practical adoption (Peng and Unluer 2024). (2) Common hyperparameter optimizers (e.g., PSO, GA) are prone to local optima in the high-dimensional, nonlinear LC³ mix space and neglect hydration kinetics (Lapeyre et al. n.d.). (3) Almost all studies are confined to the single LC³-50 framework (50% clinker substitution), lacking systematic quantification of marginal effects and interactions across a broader mix space (clinker 40–55%, calcined clay 25–35%, limestone 15–25%) (Balasubramanian and Sarangapani 2024; Vargas et al. 2025; Zunino and Scrivener 2021). These limitations cause a significant lab-engineering disconnect, reflected in prediction deviations from raw material batch variations, inability to jointly optimize strength and carbon emissions, and poor interpretability that undermines engineer trust.

To address these limitations, this study proposes a CPO-XGBoost framework for predicting LC³ paste compressive strength. Unlike conventional algorithms (e.g., PSO, GA), CPO dynamically balances exploration and exploitation via dual-stage defense: visual/sound defense for global exploration (avoiding premature convergence) and scent/physical attack with a scent diffusion factor (δ) and convergence speed factor (α) for local exploitation. CPO adaptively switches between the two phases based on the normalized fitness improvement rate, avoiding local optima and enhancing robustness across initial populations—particularly advantageous for the high-dimensional, multimodal LC³ mix optimization.

2. Materials and methods

2.1. Materials

Portland cement clinker (P·I 42.5 grade) with specific surface area of 300–500 m²/kg was used. Calcined clay was produced from kaolinite-rich raw clay calcined at 700–850 °C, with specific surface area of 10.5–23.0 m²/g (BET) and lime consumption of 450–620 mg/g (R³ test). Limestone powder (CaCO₃ ≥ 95%) had specific surface area of 300–800 m²/kg. Gypsum (natural dihydrate or FGD) had specific surface area of 300–600 m²/kg. Tap water conforming to JGJ 63-2006 was used as mixing water.

2.2. Preparation and testing methods

LC³ cement pastes were prepared by mixing cement clinker, calcined clay, limestone powder, and gypsum according to predetermined proportions, with water-to-binder ratios ranging from 0.3 to 0.5. The fresh paste was cast into molds, cured under moist conditions (20 ± 1 °C, RH ≥ 90%) for 24 hours, then demolded and stored in a water tank at 20 ± 1 °C until testing ages (1, 3, 7, 28, and 90 days). Compressive strength was measured using a compression testing machine. The preparation procedure is schematically illustrated in Figure 1.

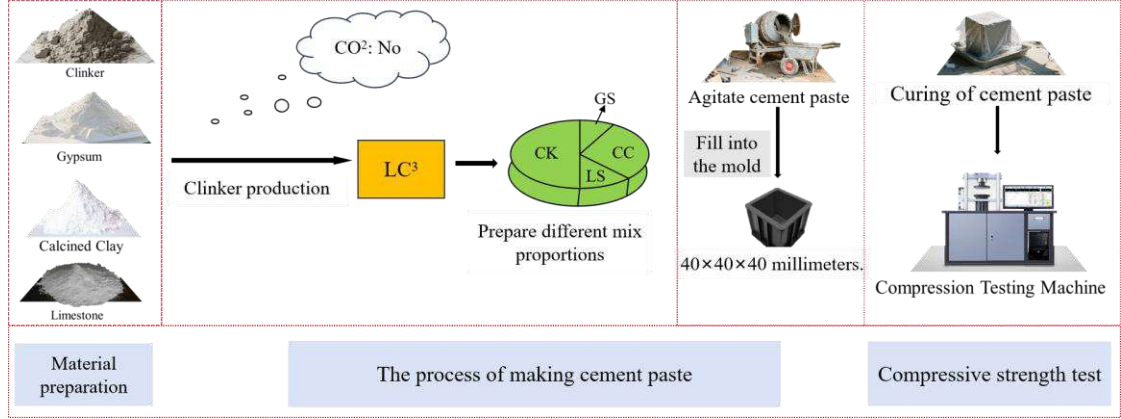


Figure 1. Schematic diagram of LC³ cement paste preparation.

2.3. Machine learning models

XGBoost involves many hyperparameters (e.g., `max_depth`, `learning_rate`, `n_estimators`). Manual tuning is inefficient, and grid/random search is computationally expensive or prone to local optima. To address this, we propose CPO-XGBoost, which mimics crested porcupine defense strategies: (1) visual/sound defense (exploration) expands the search space via random vectors; (2) scent/physical attack (exploitation) fine-tunes hyperparameters using scent diffusion factor (δ) and convergence speed factor (α). K-fold cross-validation is used to reduce overfitting and subjective bias. The workflow is shown in Figure 2.

CPO settings: population size = 30, maximum iterations = 100, δ decreases linearly from 0.9 to 0.2, $\alpha = 0.5$. XGBoost search ranges: `max_depth` $\in [3, 10]$, `learning_rate` $\in [0.01, 0.3]$, `n_estimators` $\in [100, 500]$, `subsample` $\in [0.6, 1.0]$, `colsample_bytree` $\in [0.6, 1.0]$, `min_child_weight` $\in [1, 10]$, `gamma` $\in [0, 0.5]$. Other parameters use Scikit-learn defaults. Termination: max iterations or no improvement for 20 consecutive iterations.

The mathematical formulation of CPO follows the original work by Abdel-Basset et al. (Abdel-Basset et al. 2024). The algorithm mimics four defense strategies of the crested porcupine, where the first two (visual and sound defense) correspond to global exploration, and the latter two (scent defense and physical attack) correspond to local exploitation. The position of the i -th search agent (i.e., a set of XGBoost hyperparameters) at iteration t is denoted as X_t^i . The exploration phase employs a random switch between visual defense and sound defense to avoid premature convergence. In the exploitation phase, the scent diffusion factor δ and the convergence speed factor α are defined as:

$$\delta = \exp(-t / T_{\max}) \quad (1)$$

$$\alpha = 1 - (t / T_{\max}) \quad (2)$$

where $T_{\max}$ is the maximum number of iterations. The scent defense mechanism updates the position as:

$$X_{t+1}^i = X_t^i + \delta \cdot (X_t^i - X_{\text{rand}}) + \alpha \cdot (X_{\text{best}} - X_t^i) \quad (3)$$

where X_{rand} is a randomly selected agent and X_{best} is the current best agent (global optimum). This update rule combines an exploitative move toward X_{best} and a diversification term driven by δ , allowing the algorithm to finely tune the XGBoost hyperparameters without being trapped in local optima. The

complete pseudo-code and parameter settings are available in the original publication (Abdel-Basset et al. 2024).

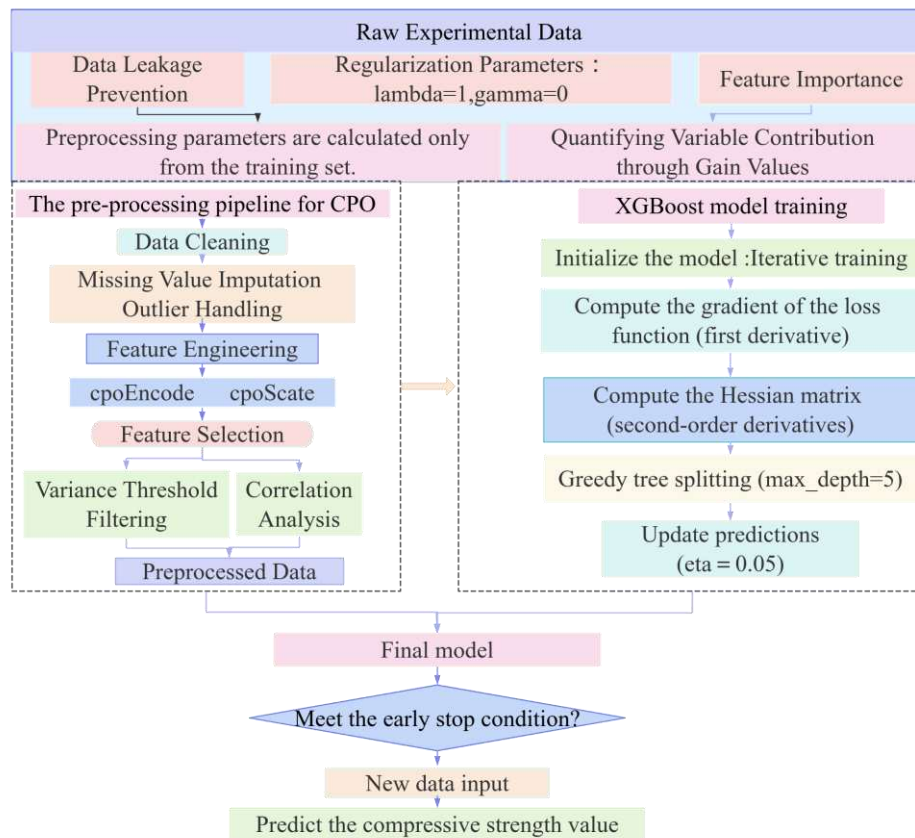


Figure 2. Schematic diagram of CPO-XGBoost algorithm principle.

To scientifically validate the effectiveness of the CPO-XGBoost model, this study extends beyond the application of a single algorithm by systematically selecting five categories of machine learning algorithms as performance benchmarks for comparison. These comparative models encompass diverse algorithmic paradigms, ensuring a comprehensive evaluation. The fundamental principles of each algorithm are summarized in Table 1.

Table 1 Mechanisms and functions of the comparative algorithms.

Algorithm Type	Model Name	Fundamental Principle	Role in This Study
Traditional Ensemble Learning	XGBoost	Gradient Boosting Decision Tree	Serves as the baseline model to validate the necessity of CPO optimization.
Bio-inspired Optimization	KOA-XGBoost	Kepler Optimization Algorithm	Compares the effectiveness of different bio-inspired strategies.
Hybrid Optimization	SSA-CatBoost	Sparrow Search Algorithm optimizes CatBoost	Verifies the generalizability of the optimization algorithm.
Neural Network	WOA-RBF	Whale Optimization Algorithm optimizes Radial Basis Function network	Represents the performance of neural network approaches.
Gradient	GBTD	Gradient Boosting Decision	Provides a comparison with traditional

Boosting	Tree	gradient boosting methods.
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To comprehensively evaluate the performance of the proposed CPO-XGBoost model, five representative algorithms from distinct machine learning paradigms were selected as benchmarks. Specifically: (i) XGBoost represents traditional ensemble learning without metaheuristic optimization, serving as a baseline to verify the necessity of hyperparameter tuning; (ii) KOA-XGBoost (Kepler Optimization Algorithm) represents a bio-inspired optimizer with a different search mechanism, allowing comparison of optimization effectiveness; (iii) SSA-CatBoost (Sparrow Search Algorithm optimized CatBoost) represents a hybrid optimization approach applied to another boosting algorithm, testing the generalizability of optimization strategies; (iv) WOA-RBF (Whale Optimization Algorithm optimized Radial Basis Function network) represents neural network-based models, assessing cross-architecture performance; and (v) GBTD (Gradient Boosting Decision Tree) represents a standard gradient boosting method without any optimization, providing a reference for the improvement achieved by CPO. This diverse selection ensures a rigorous and fair comparison across different algorithmic families.

For fair comparison, all baseline models (XGBoost, KOA-XGBoost, SSA-CatBoost, WOA-RBF, GBTD) were optimized using their respective default hyperparameter tuning strategies (grid search for XGBoost and GBTD, and built-in metaheuristic searches for KOA-XGBoost, SSA-CatBoost, WOA-RBF) with the same 10-fold cross-validation as CPO-XGBoost, and the detailed configurations are listed in Table 2.

Table 2. Hyperparameter configurations for all benchmark models.

Model	Optimizer	Search Space for Base Model	Optimizer Settings	Note
CPO-XGBoost	CPO	max_depth $\in$ [3,10]; learning_rate $\in$ [0.01,0.3]; n_estimators $\in$ [100,500]; subsample $\in$ [0.6,1.0]; colsample_bytree $\in$ [0.6,1.0]; min_child_weight $\in$ [1,10]; gamma $\in$ [0,0.5]	Population size = 30; Max iterations = 100; δ decreases from 0.9 to 0.2; $\alpha = 0.5$	Same as in manuscript
KOA-XGBoost	KOA (Kepler Optimization Algorithm)	Identical to CPO-XGBoost	Population size = 30; Max iterations = 100; Other KOA parameters as per original paper [18]	Search space kept identical for fair comparison
SSA-CatBoost	SSA (Sparrow Search Algorithm)	depth $\in$ [3,10]; learning_rate $\in$ [0.01,0.3]; n_estimators $\in$ [100,500]; l2_leaf_reg $\in$ [1,10]; bagging_temperature $\in$ [0,1]	Population size = 30; Max iterations = 100; Other SSA parameters as per original paper	CatBoost-specific parameters; ranges chosen to match complexity
WOA-RBF	WOA	hidden_layer_sizes $\in$ [50,200]; alpha	Population size	RBF network has

RBF	(Whale Optimization Algorithm)	(regularization) $\in [0.0001, 0.1]$; learning_rate_init $\in [0.001, 0.01]$	= 30; Max iterations = 100; Other WOA parameters as per original paper	fewer hyperparameters; search space defined for fair comparison
XGBoost	Grid Search	max_depth $\in [3, 5, 7, 10]$; learning_rate $\in [0.01, 0.05, 0.1, 0.3]$; n_estimators $\in [100, 200, 500]$; subsample $\in [0.6, 0.8, 1.0]$	/	Coarse grid*
GBDT	Grid Search	max_depth $\in [3, 5, 7]$; learning_rate $\in [0.05, 0.1, 0.2]$; n_estimators $\in$ [100, 200]	/	Standard GBDT implementation*

Note: * A coarser discrete grid was used for XGBoost and GBDT to limit computational cost. The continuous search space of CPO-XGBoost may contribute partially to its performance advantage. See main text for detailed discussion.

To ensure transparency and reproducibility, the detailed hyperparameter search spaces and optimizer settings for all benchmark models are provided in Table 2. Where the base model architecture differed fundamentally (e.g., RBF vs. tree-based models), search ranges were designed to be as comparable as possible in terms of model complexity. All optimization algorithms (CPO, KOA, SSA, WOA) were run with the same population size (30) and maximum iterations (100) to ensure a fair comparison.

3. Data description and variable analysis

3.1. Data description

Machine learning algorithms were used to process and clean the experimental data. The cleaned dataset was then used for predictive modeling. To investigate the influence of component contents on LC³ compressive strength, the dataset was split into training and testing sets. The feature variables were T (age), w/b, CK (clinker), GS (gypsum), CC (calcined clay), LS (limestone), SSA1–SSA4 (specific surface areas of clinker, gypsum, calcined clay, and limestone, respectively), and the target variable was CS (compressive strength). Statistical analysis of each variable is presented in Table 3. To mitigate data variability, Min-Max normalization was applied. Feature correlation analysis (Table 3) is crucial for understanding relationships with strength and selecting the optimal prediction model.

Table 3 Statistical analysis of compressive strength data variables.

	mean	std	min	25%	50%	75%	max
CK (%)	51.5070	12.0627	18.8000	50.0000	50.7000	54.0000	95.0000
GS (%)	3.2369	2.4196	0.0000	0.2000	5.0000	5.2000	7.8600
CC (%)	28.7451	7.7705	0.0000	29.4000	29.4000	30.0000	53.3000
LS (%)	15.0199	7.2888	0.0000	14.7000	14.7000	15.0000	60.0000
T (days)	20.7701	28.1890	1.0000	3.0000	7.0000	28.0000	90.0000
w/b	0.4303	0.0542	0.3000	0.4000	0.4000	0.5000	0.5000
SSA1 (m ² /kg)	401.20	61.500	300.00	350.00	400.00	450.00	500.00
SSA2 (m ² /kg)	452.30	98.700	300.00	380.00	450.00	520.00	600.00
SSA3 (m ² /g)	16.800	3.5000	10.500	14.000	16.800	19.500	23.000
SSA4 (m ² /kg)	553.40	148.90	300.00	450.00	550.00	650.00	800.00
CS (MPa)	34.1971	19.5610	1.8669	19.6700	33.2610	46.6152	95.0854

The dataset includes a small number of extreme mix designs (e.g., CK up to 95%, CC or LS at 0%) to span the full input space, but the model's recommendations are based on the data-dense regions relevant to practical LC³ production.

3.2. Data visualization

Generally, explanatory variables in multiple regression are correlated. If the correlation coefficient is too high (positive or negative), it becomes difficult to distinguish their individual effects on the response without a sufficiently large sample size, which can lead to poor estimation of partial regression coefficients (Hosseinzadeh et al. 2024). To avoid inputting similar features and overfitting, the Pearson correlation coefficient was used (Chen et al. 2023). An absolute Pearson correlation > 0.80 indicates interdependency (multicollinearity), which may degrade model performance and stability (Warne and Burningham 2019). Figure 3 presents the Pearson correlation heatmap. As shown, all correlations between variables are below 0.8, consistent with practical expectations.

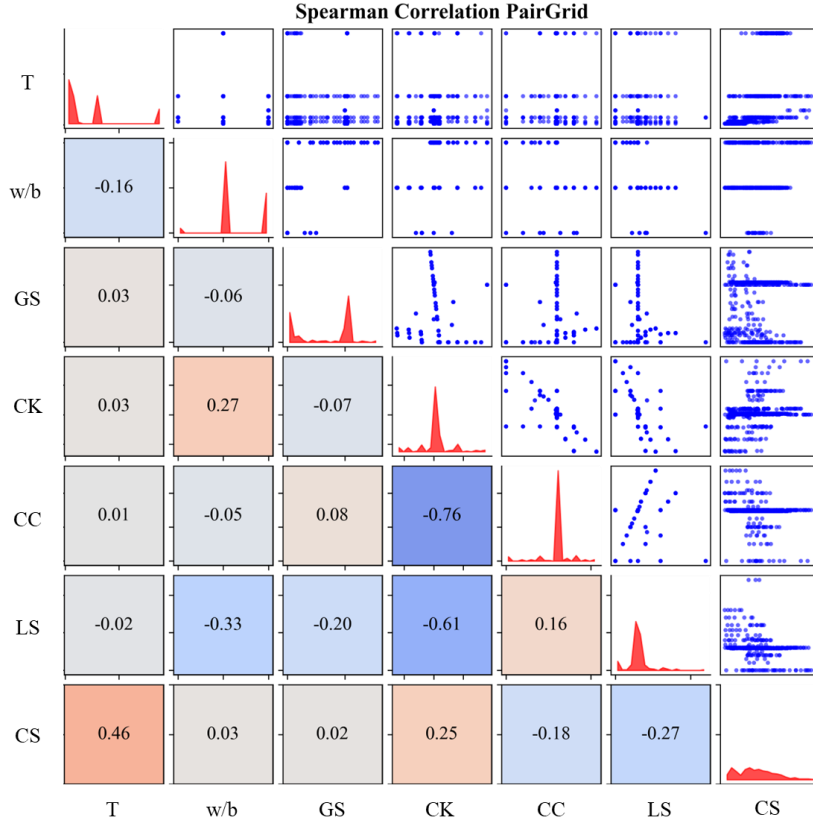


Figure 3. Heat map of correlation coefficients.

3.3. Data Preprocessing

Common data preprocessing methods include normalization and standardization. In this study, Min-Max Normalization was employed, which linearly maps data to the range $[0, 1]$. This method calculates the minimum and maximum values of the data and performs linear mapping to the specified range to reduce data variability and enhance model robustness. Its calculation formula is as follows (Jain et al. 2005):

$$x' = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \quad (4)$$

In this formulation, x represents the original data point, $x_{\min}$ denotes the minimum value in the dataset, $x_{\max}$ indicates the maximum value, and x' corresponds to the normalized value confined to the range $[0,1]$.

3.4. Model evaluation metrics

This study employs RMSE, MSE, MAE, Explained Variance Score, and R^2 (0–1, higher is better) to evaluate model performance. RMSE and MAE range from 0 to ∞ (Chai and Draxler 2014; Quan Tran et al. 2022).. The mathematical expressions are as follows:

$$R^2 = \frac{\sum_{k=1}^N (q_{0,k} - \bar{q}_0)(q_{t,k} - \bar{q}_t)}{\sqrt{\sum_{k=1}^N (q_{0,k} - \bar{q}_0)^2 \sum_{k=1}^N (q_{t,k} - \bar{q}_t)^2}} \quad (5)$$

$$MAE = \frac{1}{N} \sum_{k=1}^N \left| \frac{q_{0,k} - q_{t,k}}{q_{0,k}} \right| \quad (6)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{k=1}^N (q_{0,k} - q_{t,k})^2} \quad (7)$$

$$MSE = \frac{1}{N} \sum_{k=1}^N (q_{0,k} - q_{i,k})^2 \quad (8)$$

Where: N represents the number of samples; q_0 denotes the actual value; $\bar{q}_0$ indicates the mean of the actual values; q_t represents the predicted value; and $\bar{q}_0$ signifies the mean of the predicted values.

4. Results

4.1. Interpretability analysis

This study employed SHAP (SHapley Additive exPlanations) analysis to evaluate the importance of each variable. Figure 4(a) depicts the impact of the 10 input variables on the output variable, while Figure 4(b) presents the relative importance ranking of these 10 input variables. In these figures, features with higher sample values are represented by darker red shades, whereas features with lower sample values are indicated by darker blue shades (Marcílio and Eler 2020; Parsa et al. 2020). The features are arranged from top to bottom, indicating their relative importance in predicting the outcome (Nandi Buddhadev and Das Subhasish 2025; Zhang et al. 2023). This ranking is consistent with the feature importance order shown in Figure 4(b). For compressive strength prediction, the top five most critical features based on Shapley values are T, GS, SSA1, w/b, and SSA3.

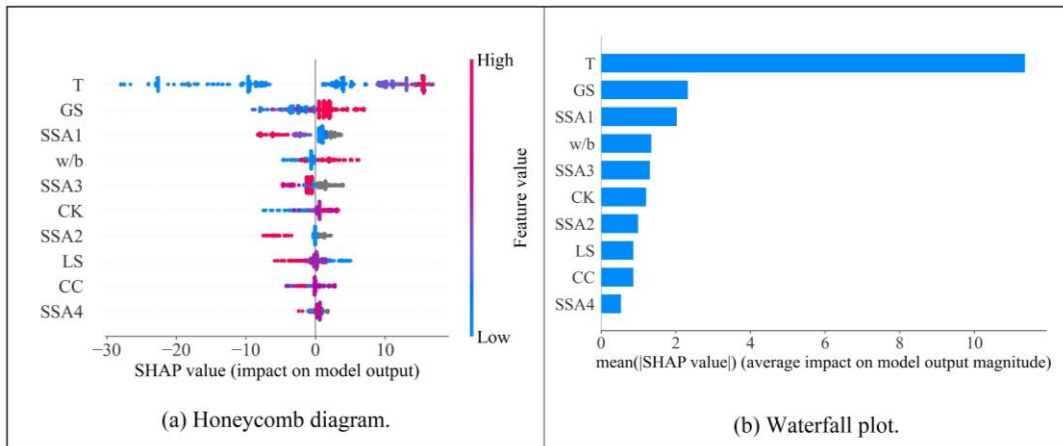


Figure 4. SHAP analysis for compressive strength prediction of LC³ paste. (a) Feature importance ranking (mean SHAP value). (b) Beeswarm plot showing the impact of feature values (Red: high, Blue: low) on the SHAP value, which represents the marginal contribution to predicted strength (MPa).

The feature importance ranking in Fig. 4(a) shows T, GS, SSA1, w/b, and SSA3 as the top five features. The beeswarm plot (Fig. 4(b)) reveals direction and non-linear marginal effects. For gypsum (GS), low GS values (blue dots) lie on the negative SHAP side (detrimental), while high GS values (red dots) cluster on the positive side, with strongest contributions near 4–5 %. This indicates a threshold: below 2–3 % GS, marginal effect negative; between 3 % and 5 %, positive; beyond 5 %, plateau.

Notably, GS and clinker specific surface area (SSA1) rank among the top three features, surpassing clinker content (CK)—counter-intuitive for traditional PC but characteristic of LC³. The dominance of GS underscores the critical role of sulfate balance. Metakaolin from calcined clay provides additional alumina, demanding precise sulfate supply to form monosulfoaluminate and ettringite. Insufficient GS (<2–3 %) causes uncontrolled aluminate hydration, flash setting, and a porous microstructure; excess GS (>5 %) risks delayed ettringite formation and expansion. Thus, GS acts as a ‘chemical regulator’ amplified in LC³.

The high importance of SSA1 suggests that in LC³ blends with diluted clinker (40–55 %), clinker hydration kinetics become rate-limiting. This aligns with classical theories (e.g., Avrami equation): C-S-H nucleation and growth rate are proportional to clinker specific surface area, an effect that becomes rate-determining under significant dilution. Finer clinker (higher SSA1) provides more surface area for water contact, accelerating early hydration and compensating for reduced clinker quantity. Hence, optimising clinker fineness is more effective for early strength than marginally increasing clinker content within the 40–55 % range. The dominant importance of curing age (T) is expected, reflecting progressive hydration and pozzolanic reactions as primary strength drivers.

4.2. Analysis of prediction results

4.2.1. Model training

The dataset was split by stratified random sampling into training (80%) and test (20%) sets (Dai et al. 2024; Rosa et al. 2022). The training set was used for iterative parameter optimization via backpropagation, while the test set served as an independent validation for generalization. Ten-fold cross-validation was applied to assess model stability and reduce partition bias. CPO-based hyperparameter tuning was performed exclusively on the training set using the same ten-fold cross-validation. The optimal hyperparameters were then used to train a final model on the entire training set, which was evaluated once on the test set. This strict separation prevents data leakage and ensures unbiased generalization estimation.

During the model training process, the CPO-XGBoost framework (CPO-optimized XGBoost) demonstrated superior goodness-of-fit (R^2) and higher accuracy (reflected by lower MSE, MAE, and RMSE values) compared to the other four machine learning algorithms. Similarly, Philip and Marakkath (2025) employed particle swarm optimization to optimize XGBoost for predicting the compressive strength of geopolymer concrete (Philip and Marakkath 2025), while Muhammad Zeshan Akber et al. (2024) utilized tree-structured Parzen estimator to optimize XGBoost for predicting the compressive strength of conventional concrete (Akber et al. 2024). Both studies confirmed the effectiveness of hyperparameter optimization strategies in improving prediction accuracy compared to traditional tuning methods. Furthermore, Chen et al. (2025) applied an improved crown porcupine optimizer to XGBoost for traffic accident severity prediction (Chen et al. n.d.), further extending the applicability of such optimization algorithms in engineering prediction tasks. Collectively, these studies and the present

experiment demonstrate that XGBoost frameworks based on metaheuristic or Bayesian optimization can effectively enhance model generalization in prediction tasks within civil engineering and related fields.

4.2.2. Model testing

The predictive performance of the six models was evaluated using the metrics in Section 3.4 (R^2 , MSE, MAE, RMSE), with results in Table 4. CPO-XGBoost achieved the highest R^2 of 0.938 on the test set. The training R^2 was 0.945, only 0.007 higher, indicating no significant overfitting. This small discrepancy is acceptable, owing to the inherent data split variability, the 10-fold cross-validation, and XGBoost's regularization mechanisms (e.g., gamma, min_child_weight, subsample). The close training-test consistency demonstrates robust generalization to unseen data. Table 4 lists all six models' metrics, and Figure 5 shows the test scatter plot. The solid black line represents the ideal baseline (perfect prediction, $R^2 = 1$, zero error).

Table 4 Statistical table of training performance and test performance results of CS related data sets.

	R^2		MAE		RMSE		MSE	
	Train	Test	Train	Test	Train	Test	Train	Test
CPO-XGBoost	0.945	0.938	2.571	3.629	4.573	4.864	20.914	23.656
SSA-CatBoost	0.851	0.830	4.753	5.534	7.554	8.025	57.065	64.407
KOA-XGBoost	0.844	0.820	5.113	5.809	7.719	8.249	59.584	60.044
GBTD	0.814	0.821	5.839	5.920	8.431	8.220	71.081	67.559
XGBoost	0.809	0.811	6.335	6.303	8.552	8.447	73.141	71.358
WOA-RBF	0.778	0.789	6.385	6.687	9.215	8.910	84.912	79.391

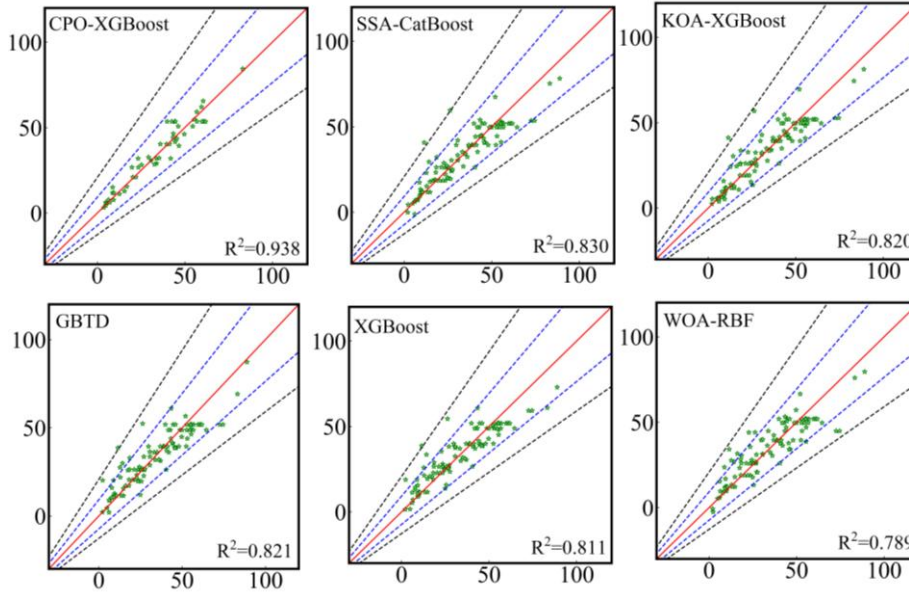


Figure 5. Scatterplot of test performance of CS related data sets.

4.2.3. Model comparison

The Taylor diagram provides a statistical summary of model performance through three key metrics: the correlation coefficient, root-mean-square error (RMSE), and normalized standard deviation. This visualization tool enables a comparative assessment of multiple model ensembles by plotting the standard deviation on orthogonal axes, representing the correlation coefficient via radial lines, and displaying the

RMSE values using semicircular iso-contours (Sobuz et al. 2025; Wang et al. 2022). Figure 6 presents a Taylor diagram constructed from the performance of the six developed ML models in predicting the CS-related dataset. The closer a point is to the reference point in the diagram, the superior the model's predictive performance, thereby allowing for the comparison of their predictive capabilities and the selection of the optimal ML model. The reference point in the diagram represents an ideal model with an R^2 value of 1 and zero error, while the position of each point indicates the correlation between the actual model and the reference model (Khan et al. 2025). CPO-XGBoost consistently achieved lower RMSE and higher R^2 than all other models across all 10 cross-validation folds, with negligible standard deviation (e.g., R^2 SD < 0.015), indicating that the improvement is robust and not due to random data splits. It should be noted, however, that the baseline models XGBoost and GBTD were tuned using a coarse grid search (Table 2), whereas CPO-XGBoost explored a continuous hyperparameter space. This difference in search space granularity may partially contribute to the observed performance gap. While the coarser grid for baseline models may partially understate their potential, the metaheuristic approach offers a practical advantage in high-dimensional nonlinear problems where grid search becomes computationally prohibitive.

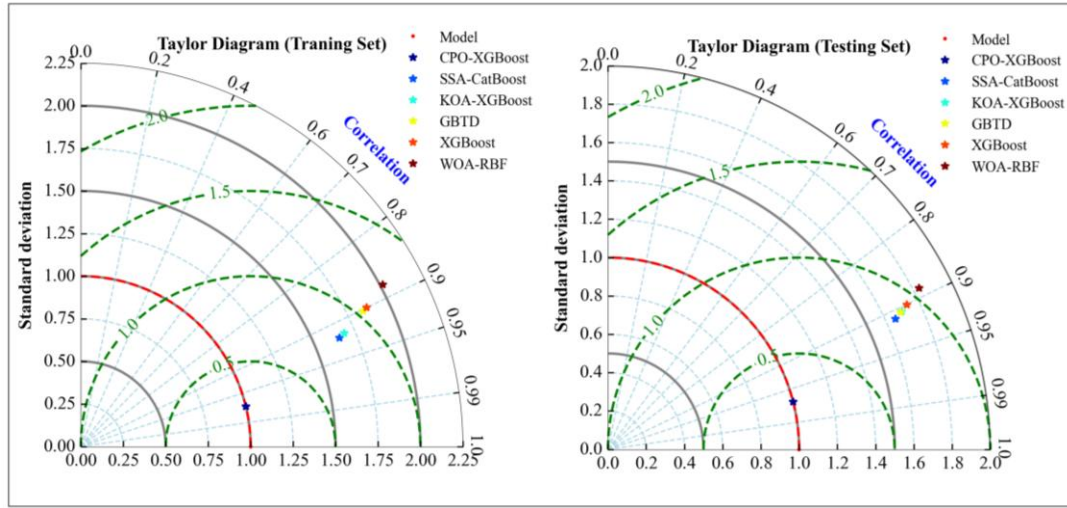


Figure 6. Model comparison Taylor diagram.

4.3. Partial dependence plot (PDP)

Figure 7 presents the Partial Dependence Plots for compressive strength (CS) input variables. The reliability of PDP curves depends on data density. The most reliable regions are: calcined clay (CC) 25–40 %, clinker (CK) 40–55 %, limestone (LS) 15–25 %, and gypsum (GS) 3–5 %. In sparse-data regions (e.g., CC < 25 % or > 40 %), the curves represent model extrapolations and should be interpreted as hypotheses.

Clinker (CK): When CK ranges from 20 % to 70 %, dependence increases with CK ratio and converges near 40–55 %. At 40 % CK, strength foundation is weak; above 55 %, supplementary materials become too low, reducing marginal benefits.

Calcined clay (CC): Within the data-dense region (25–40 %), the PDP rises rapidly near 30 % and plateaus around 35 %. In the reliable range (25–35 %), the marginal effect is positive; beyond 35 % (up to 40 %), it decreases because excessive clay may interfere with early hydration and ettringite stability. Recommended CC: 25–35 %.

Gypsum (GS): The PDP is non-monotonic: slightly negative below 2 %, rising steadily from 2 % to

5 % (peak at 4–5 %), then plateauing. Below 3 %, insufficient sulfate leads to uncontrolled aluminate hydration; within 3–5 %, the marginal effect is clearly positive. Beyond 5 %, the benefit plateaus, and higher sulfate risks delayed ettringite formation. Optimal GS: 3–5 %.

Limestone (LS): Dependence first decreases then increases within 0–40 %, leveling off between 20 % and 30 %. Below 15 %, negative correlation due to limited carboaluminate formation and poor ettringite stability. Above 25 %, excessive limestone dilutes active components. Recommended LS: 15–25 %.

Water-to-binder ratio (w/b): Marginal contribution is slightly positive from 0.30 to 0.40 (improved workability and hydration), but becomes negative from 0.40 to 0.50 (dilution and porosity dominate).

Curing age (T): Longer curing time correlates with faster strength growth, leveling off after 30 days, consistent with typical LC³ strength development.

Based on the SHAP and PDP analyses, the optimal composition range for LC³ cement paste is: clinker 40–55 %, calcined clay 25–35 %, limestone 15–25 %, and gypsum 3–5 %. These recommendations are based on specific experimental conditions (standard curing, w/b 0.3–0.5, defined raw materials). For practical applications, adjustments should consider local raw material characteristics and grinding fineness; localized small-scale trials are recommended. When applying to concrete, additional factors (aggregate type, superplasticizer compatibility, ITZ effects) may influence strength; pilot-scale validation is strongly advised.

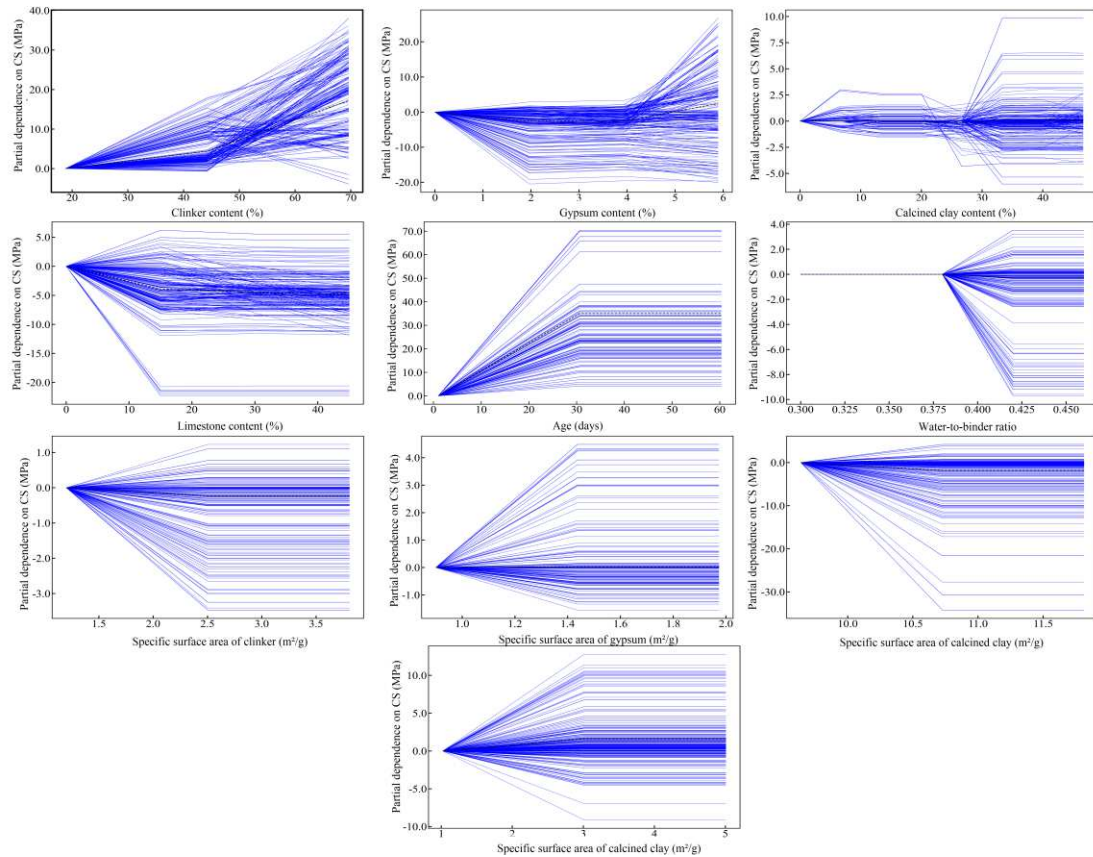


Figure 7. Average Partial Dependence Plots (PDPs) for key components of LC³ paste.

4.3.1. Implementation of the system architecture

To address practical challenges (raw material variability, multi-objective optimization, and code compliance), an intelligent design system was developed (Fig. 8). Its core functions are:

- (1) Front-end: Users input target strength and curing age; the system outputs real-time mix

visualizations and strength curves.

(2) Model computation: The pre-trained CPO-XGBoost model predicts compressive strength.

(3) Optimization engine: When the deviation between predicted and measured strength exceeds 5 %, an NSGA-II algorithm triggers bias correction using the latest lab results without full model retraining.

The system operates within validated mix ranges: clinker 40–55 %, calcined clay 25–35 %, limestone 15–25 %, gypsum 3–5 %. Outputs require small-scale validation before engineering use.



Figure 8. Intelligent design system for LC³ cement mix proportions.

4.3.2. Specification compliance

To ensure engineering reliability, the system strictly constrains input parameters within validated ranges: clinker 40–55 %, calcined clay 25–35 %, limestone 15–25 %, gypsum 3–5 %, w/b 0.3–0.5, and curing age 1–90 days. If the deviation between measured and predicted strength exceeds 5 %, the system triggers a re-optimisation and recommends three alternative mix designs. The interaction workflow is as follows: (1) users input target strength and raw material constraints; (2) the system returns predicted strength, mix proportions, and SHAP-based feature contributions; (3) if lab test deviations exceed 5 %, the system issues a warning and suggests optimised alternatives.

4.4. Carbon reduction potential analysis

Based on the optimal proportion range for LC³ identified in this study (e.g., Clinker (CK) 40–55%, Calcined Clay (CC) 25–35%, Limestone (LS) 15–25%, Gypsum (GS) 3–5%), the theoretical range of carbon emissions was calculated, and the reduction potential was analyzed by comparing it with traditional Ordinary Portland Cement (OPC) (with 100% clinker). The specific methodology and rationality assessment are as follows:

Carbon Reduction Rate Calculation Formula:

$$\text{Emission reduction rate} = \left(1 - \frac{\text{LC3 CO}_2\text{emission}}{\text{OPC CO}_2\text{emission}} \right) \times 100\% \quad (9)$$

4.4.1. Engineering implementation roadmap

Based on the model validation results and laboratory data, the phased implementation pathway proposed in this study demonstrates the following technical feasibility: the laboratory validation phase (involving 3–5 trial mixes) ensures the agreement between model predictions and measured data; the pilot production phase (50–100 m³) verifies the scalability of the mix proportion designs; the bulk

application phase achieves intelligent management through the establishment of a mix proportion database; and regular (quarterly) model parameter updates maintain prediction accuracy. To enhance the system's adaptability, subsequent research is recommended to establish a regional model calibration mechanism, which involves periodically collecting data on local raw material characteristics (e.g., at regular six-month intervals) and focusing on key parameters such as calcined clay reactivity and limestone purity for model optimization. The design of this implementation pathway references the general validation procedures commonly adopted in cement-based material research (ASTM Committee 2018; EN 2009). Considering the specific characteristics of LC³ materials, it is further advised to supplement the raw material reactivity assessment by referring to the standard methods for determining the reactivity index of calcined clay in cement (American Society for Testing and Materials. Committee C-9 on Concrete and Concrete Aggregates 2008).

4.4.2. Determination of carbon emission factors and system boundaries

The carbon emission factors used in this study are derived from internationally authoritative databases and literature: the emission factor for clinker (CK) (0.83–0.94 kg CO₂/kg) is cited from the 'Getting the Numbers Right' database by the Global Cement Sustainability Initiative (GCSI) (Iniciative 2014); the factor for calcined clay (CC) (0.12 kg CO₂/kg) references the measured data under 700°C calcination conditions reported by Avet et al. (Avet and Scrivener 2018); the emission factors for gypsum (GS) and limestone (LS) are obtained from the life cycle assessment (LCA) studies by Hammond et al. (Hammond and Jones 2008) and Marmier (Marmier 2023), respectively. For specific values, please refer to Table 5. This study adopts a gate-to-gate system boundary, accounting for CO₂ emissions directly from the production (calcination) of clinker, calcined clay, limestone, and gypsum. Emissions from raw material extraction, transportation, and final grinding are not included due to data availability constraints and to maintain consistency with the source literature (Avet and Scrivener 2018; Hammond and Jones 2008; Iniciative 2014; Marmier 2023). Therefore, the reported carbon reduction rates represent direct process emissions only and are not directly comparable to full LCA studies.

The carbon emission factors used in this study are generalized literature values. In practice, they vary with production conditions and region (e.g., clinker factor ranges from 0.81 kg CO₂/kg for modern preheaters to 1.05 kg CO₂/kg for shaft kilns (Iniciative 2014)). Local data should be used for real applications.

Table 5 Carbon emission factors and references for each raw material.

Material	Carbon Emission Factor
CK	0.83-0.94 kg CO ₂ /kg (Iniciative 2014)
CC	0.12 kg CO ₂ /kg (Avet and Scrivener 2018) (under 700°C calcination condition)
GS	0.08-0.12 kg CO ₂ /kg (Hammond and Jones 2008)
LS	0.02-0.04 kg CO ₂ /kg (Marmier 2023)

Based on these factors, the calculated CO₂ emission intensity of LC³ is 0.435–0.540 kg CO₂/kg (Fig. 9). Compared to ordinary Portland cement, LC³ achieves a carbon reduction of 41.9–53.2 % (Table 6, Fig. 9), which exceeds the ~40 % reduction reported for LC³-50 (50 % clinker) by Scrivener et al. (Scrivener et al. 2018). The reduction is nonlinear: as clinker drops below 40 %, the marginal benefit diminishes because supplementary materials (e.g., calcined clay) contribute more emissions (from 7 % to 10 % when clay increases from 25 % to 35 %). This provides a conservative yet practical basis for mix optimization.

Table 6 Table of carbon emission ranges corresponding to mixing ratios.

Scenario	CK (%)	CC (%)	LS (%)	GS (%)	CO ₂ emission (kg/kg)	Reduction Rate
Lower-bound (Low-carbon)	40	35	25	5	0.435	53.2%
Recommended Median	47.5	30	20	4	0.487	47.6%
Upper-bound (Low-carbon)	55	25	15	3	0.540	41.9%
Traditional OPC	100	0	0	0	0.93	0%

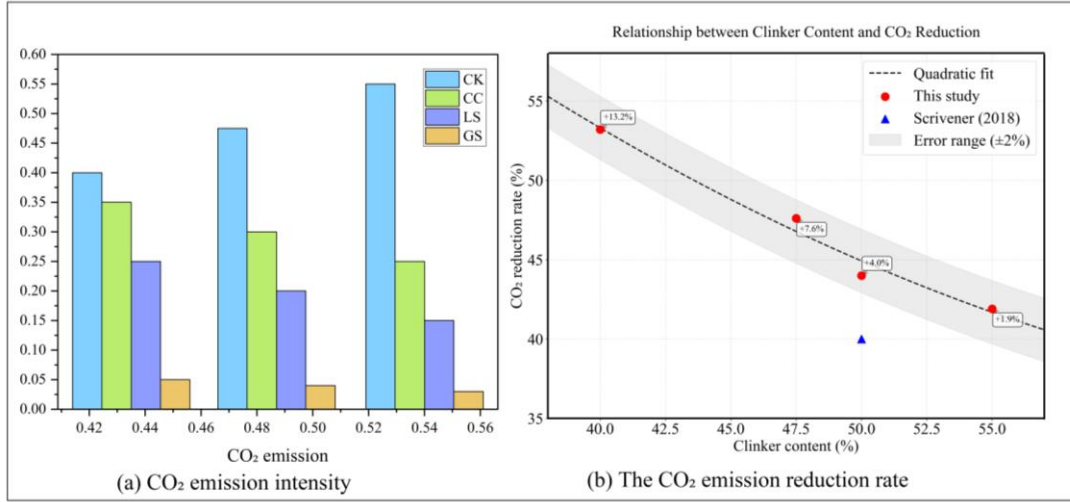


Figure 9. Carbon emission visualization data chart.

4.4.3. Impact of uncertainty in carbon emission factors

The carbon emission factors used in this study are subject to three main uncertainties. First, regional disparities in energy efficiency and production technology can cause clinker emission factors to vary significantly (e.g., developing countries often have 15–25% higher intensities). Second, technological evolution (e.g., electrochemical clinker recycling) may reduce clinker factors from ~ 0.9 to below $0.5 \text{ kg CO}_2/\text{kg}$ in the future. Third, the gate-to-gate system boundary excludes upstream (mining, transport) and downstream processes; full life-cycle emissions are higher. Future work should incorporate regionalised databases and full LCA.

4.5. Limitations and future work

This study has three main limitations. First, the model and optimal mix ranges are derived from LC³ paste under standard curing; application to concrete requires validation with aggregates and superplasticizers. Second, the dataset was generated from a single laboratory; industrial generalization needs further testing. Third, the carbon emission analysis is based on a gate-to-gate system boundary using literature-derived, geographically generalized emission factors. This simplification does not account for regional variations in energy grids, transportation distances, or raw material extraction. A full cradle-to-gate Life Cycle Assessment (LCA) is necessary for a more accurate and location-specific environmental impact quantification and is a key direction for our future work.

5. Conclusion

This study systematically investigated the compressive strength prediction and low-carbon optimization design of Limestone Calcined Clay Cement (LC³) through integrated experimental and machine learning approaches. The main conclusions are as follows:

- (1) The CPO-XGBoost model achieves excellent compressive strength prediction for LC³ paste (test

$R^2 = 0.938$), outperforming XGBoost, SSA-CatBoost, and other benchmark algorithms. Ten-fold cross-validation confirms its strong generalization and robustness.

(2) SHAP and PDP analyses reveal the nonlinear marginal effects of each component. The optimal mix ranges are: clinker 40–55 %, calcined clay 25–35 %, limestone 15–25 %, and gypsum 3–5 %.

(3) Carbon emission analysis shows that the optimised LC³ mix reduces CO₂ emissions by 41.9–53.2 % compared to ordinary Portland cement (OPC).

(4) A prototype intelligent design system (Python/Streamlit) is developed for real-time strength prediction and low-carbon mix optimisation. Industrial application requires further validation with field production data.

Declarations

Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contributions

Jinpeng Dai: Conceptualization, Methodology, Project administration, Funding acquisition, Writing - Original Draft, Validation, Resources. Fanghui Lu: Conceptualization, Supervision, Software, Investigation. Riccardo Maddalena: Formal analysis, Data Curation. Xuwei Dong: Writing - Review & Editing. Yuhu Qi: Investigation.

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Data Availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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