Prediction the Chloride Ion Permeation Coefficient of Concrete Based on A Hybrid Intelligent Algorithm

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Abstract Chloride ion penetration resistance (CIPR) is a critical concern in engineering to ensure the long-term durability of concrete structures, accurately predicting concrete CIPR is essential for designing the appropriate mix ratio. The rapid chloride migration (RCM) test is the most commonly used experimental method, typically employed to measure CIPC. To efficiently and accurately predict the CIPR of concrete, a Bayesian Optimization (BO)-Light Gradient Boosting Machine (LGBM) model is developed. Through this research, it can be concluded that (1) BO can effectively search and optimize the hyperparameters in LGBM. Within 100 iterations, BO optimization can search the hyperparameters effectively and find the optimal solution quickly.(2) BO-LGBM has a strong predictive ability, and its prediction accuracy is superior than the other three prediction models. The outcomes indicate that the application of this model has important practical significance for predicting the CIPC of concrete, optimizing the design of the concrete mix ratio and improving the durability of concrete.

Keywords Chloride ion penetration resistance; Durability of concrete; BO-LGBM; intelligent Prediction

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Introduction

Segments are essential components in shield tunnel construction. Chloride is a significant factor that triggers corrosion of steel reinforcement in shield tunnel pipe segments, thus impacting their durability. The common cause of durability failure in concrete structures is the intrusion of mediums such as gases and liquids, in other words, the permeation and diffusion of various external harmful substances like liquids, gases, and ions in concrete[1]. CIPR is the primary line of defense for ensuring concrete durability and serves as a critical evaluation indicator for its long-term performance. Scholars such as Academician Zhongwei Wu and others believe that improving the CIPR of concrete is key to enhancing its durability[2]. Consequently, studying the CIPR of concrete used in shield tunnel segments holds great significance in ensuring the safe operation of the segments and shield tunnel.

Many scholars at home and abroad have conducted experimental research on the resistance of concrete to chloride ion penetration. For example, Yanru Wang (2019) studied the water absorption and chloride diffusion rate of concrete under the coupling effect of uniaxial compressive load and freeze-thaw cycles[3]. Song Gao (2022) et al. investigated the chloride ion diffusion performance of recycled aggregate concrete[4]. Yuanzhan Wang (2020) studied the mechanical properties and chloride permeability of concrete made with fly ash and coal gangue mixture[5]. In the above studies, the rapid chloride migration (RCM) test is the most commonly used experimental method, typically employed to measure CIPC. It has the advantages of short testing time, good repeatability, and results that closely resemble actual conditions.

The aforementioned experimental studies have laid the foundation for understanding the permeability of concrete to chloride ions. However, these experiments are time-consuming, costly, and have limitations in accurately considering multiple factors and their nonlinear relationships, which restrict their practical application. With the development of artificial intelligence, machine learning methods have provided a new approach to solving complex nonlinear engineering prediction problems[6]. Machine learning algorithms (ML) possess powerful data processing capabilities and are suitable for solving complex nonlinear problems with multiple factors, making them widely used in research related to engineering.

Various machine learning algorithms, such as BP[7]，ANN[8] , and Support Vector Machine (SVM)[9] have been widely used in concrete performance prediction[10]. ANN and BP have excessive data requirements, tend to fall into local optima, and are also sensitive to initialization and hyperparameters[11]. SVM prediction algorithm is more troublesome in preprocessing data and tuning parameters, and is more sensitive to missing data[12]. LGBM algorithm significantly improves the training speed of the algorithm and picks to avoid the overfitting problem to a certain extent. Therefore, it is feasible to use the LGBM algorithm for CIPC prediction to obtain the fitness function.

Furthermore, the performance of the LGBM algorithm's predictions is directly influenced by the selection of hyperparameters. To optimize the prediction results, careful parameter tuning is required for the LGBM algorithm. Commonly used methods for optimizing the hyperparameters of LGBM include Grid Search (GS)[13], Random Search (RS)[14], and Bayesian Optimization (BO)[15]. Among these three optimization methods, GS takes too long to train[16], RS tends to fall into local optimum[17], and BO optimization is widely used to solve the parameter combination optimization problem for it finds the optimal solution of hyperparameters quickly and accurately[18, 19].

From the analysis provided, the primary research questions can be summarized as: (1) How to establish an intelligent forecasting framework for concrete CIPC? (2) How can we establish a fast and accurate nonlinear mapping relationship between concrete's CIPC and its main influencing parameters for predicting CIPC efficiently? To this end, this study presents a framework for predicting CIPC of concrete. The main contributions of this study include:

(1) BO can effectively search and optimize the hyperparameters in LGBM. Within 100 iterations, BO optimization can search the hyperparameters effectively and find the optimal solution quickly.

(2) The constructed BO-LGBM model has the best fitting effect. Compared with other prediction models, the BO-LGBM algorithm predicts the results with the smallest RMSE and MAE, and biggest R^2.

(3)A hybrid intelligent prediction framework for CIPC was developed and provided a basis for the intelligent prediction of concrete CIPC.

The implementation of this research framework is organized as follows. Part 2 introduces the BO-LGBM mixed prediction framework of the CIPC for concrete. Next, Section 3 analyzes the application of the BO-LGBM model in practical projects. The relevant studies are discussed in Section 4. Finally, Part 5 summarizes the full text and looks forward to the future work.

Methodology

The flow chart of the developed BO-LGBM prediction model of concrete CIPC is present in Figure 1.It consists of three primary steps: creating a sample dataset, building a prediction model, and evaluating the model's performance.

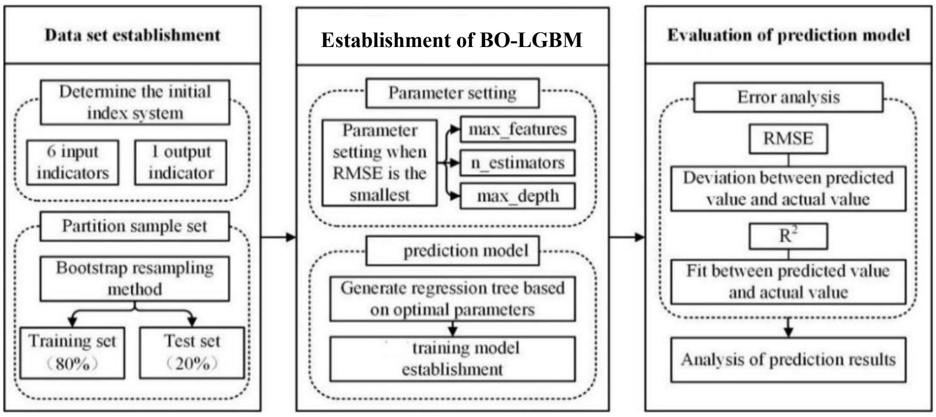


Figure 1. Flowchart of the CIPC regression model based on BO-LGBM

Dataset acquisition

Many factors affect the concrete CIPR, for instance, cement, additives, and the water-binder ratio. The relationships among these agents and the CIPC is not only a multiple nonlinear relationship but also has a great impact on the performance of concrete[20]. This paper selects the commonly used parameters that influence the CIPR of concrete[21], the output index is the CIPC, constructs an initial index system, conducts related experiments, collects statistical data, and uses the corresponding data as the original dataset.

Hyperparameter optimization

Principles of BO optimization

The BO optimization process involves two key components: the statistical model used to construct the objective function and the acquisition function utilized to determine the next sampling point. To be as close as possible to the real objective function, the BO algorithm uses Gaussian Process (GP) agent model. During cross-validation, the relationship between the chosen hyperparameters and the predicted performance can be visualized through a GP model mapping with a confidence interval for each inference. In general, calculating and adding the probability of each feature in a GP model requires constructing the covariance matrix. Eq. (1) displays the final multivariate GP model [22]:

$$P(x) = \frac{1}{(2\pi)^{\frac{n}{2}}|cov|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\mu)^T cov(x-\mu)^{-1}\right) \tag{1}$$

where μ (mean) and cov (covariance) are seen Eqs. (2) and (3):

$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i \tag{2}$$

$$cov = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)(x_i - \mu)^T \tag{3}$$

An acquisition function is employed to ameliorate for each sampling point. Expected Improvement (EI) is utilized within the acquisition function to identify the parameter with the best accuracy and designate it as the final parameter. Mathematically, this can be represented as Eq. (4)[23]:

$$EI(X_n) = (y_{best} - \mu(X_n))\phi\left(\frac{y_{best}-\mu(X_n)}{\sigma(X_n)}\right) + \sigma(X_n)\varphi\left(\frac{y_{best}-\mu(X_n)}{\sigma(X_n)}\right) \tag{4}$$

In the equation, $\phi\left(\frac{y_{best}-\mu(X_n)}{\sigma(X_n)}\right)$ represents the cumulative probability distribution, while $\varphi\left(\frac{y_{best}-\mu(X_n)}{\sigma(X_n)}\right)$ represents the probability distribution function of the standard Gaussian distribution. Here, X_n refers to the nth sampling point, and y_{best} represents the best tentative optimum within the current sample space.

LGBM hyperparameters

The settings of hyperparameters directly affect the performance of LGBM prediction models[24, 25]. Parameter tuning is essential to enhance the prediction performance of the LGBM algorithm. Herein, BO, currently widely used, is used to optimize the performance of prediction algorithm. The hyperparameters of machine learning algorithms used in this paper is given in Table 1. The first parameter is learning_rate, which controls the step size used in the gradient descent optimization. The second parameter is num_leaves, which controls the upper limit of the number of leaves allowed in each tree. The third parameter, max_depth, is chosen to determine and regulate the maximum depth of each tree in the fusion. A large learning_rate will result in the model exceeding the optimal solution, while a small one will result in slow convergence, and too high num_leaves and max_depth may result in overfitting, while too low may result in underfitting[26].

Table 1. LGBM algorithm hyperparameters

Machine Learning Algorithms	Hyperparameters to be optimized	Definition
	learning_rate	Rate of learning
LGBM	num_leaves	Number of leaves per decision tree
	max_depth	Maximum depth

BO-LGBM Prediction Algorithm

LGBM

LGBM incorporates several key concepts such as histogram algorithms, depth-constrained leaf growth strategies, support for categorical features, histogram feature optimization, gradient-based unilateral sampling techniques, multithreading optimization, and cache hit rate optimization. In the LGBM algorithm, the target value is denoted as y_i, the predicted value as $\hat{y}_i^{(t)}$, S denotes the number of leaf nodes, q denotes the structural function of the tree, and w denotes the leaf weights. The objective function of the model is given by Eq. (5)[27]:

$$Obj^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t)}\right) + \sum_{i=1}^{t}\Omega(f_i) \tag{5}$$

Expanding the objective function through Taylor's formula provides Eqs. (6), (7), (8).

$$Obj^{(t)} \cong \sum_{i=1}^{n}\left[l\left(y_i, \hat{y}_i^{(t-1)}\right) + g_i f_t(x_i) + \frac{1}{2}h_i f_t^2(x_i)\right] + \Omega(f_t) \tag{6}$$

$$g_i = \partial_{\hat{y}_i^{(t-1)}} l\left(y_i, \hat{y}_i^{(t-1)}\right) \tag{7}$$

$$h_i = \partial^2_{\hat{y}_i^{(t-1)}} l\left(y_i, \hat{y}_i^{(t-1)}\right) \tag{8}$$

In Eqs. (7), (8), and (9), the final objective function of the LGBM model is obtained by traversing all leaf nodes using the accumulation of n samples, as shown in Eq. (9):

$$Obj^{(t)} = \sum_{j=1}^{S}\left[G_j w_j + \frac{1}{2}\left(H_j + \lambda\right) w_j^2\right] \tag{9}$$

where $G_j = \sum_{i \in I_j} g_i$, $H_j = \sum_{i \in I_j} h_i$, I is the set of samples in leaf node j. The pseudo-code is shown in Table 2.

Table 2. BO-LGBM pseudo-codes

Algorithm 1: Bayesian algorithm
Input: X_i and N (maximum iterations)
Output: x
For $t = 1,2,3,\ldots,N$ **do**
  Find x,by optimizing the acquisition function over the GP:
  $x, = \arg\max x, u(x|X_{1:t-1})$
  Get a new sample $(x_t, f(x_t))$
  Augment the data $X_{1:t}$={$X_{1:t-1}, (x_t, f(x_t))$}
End

Algorithm 2: LGBM algorithm
Input: two individuals A and B
Output: whether $A\ dominates\ B$
Foreach $objective\ m$ **do**
  $better\_flag$ = $Flase$
  $A_{fitness}^{m}$ = $LGBM\ Regression\ Model(A)$
  $B_{fitness}^{m}$ = $LGBM\ Regression\ Model(B)$
  If $A_{fitness}^{m} < B_{fitness}^{m}$ **then** Assuming that higher fitness corresponds to better performance.
    Return $A\ doesn't\ dominate\ B$
  Else if $A_{fitness}^{m} > B_{fitness}^{m}$ **then**
    $better\_flag$ = $True$
  End
End
If $better\_flag$ = $True$ **then**
  Return $A\ dominates\ B$
Else
  Return $A\ doesn't\ dominate\ B$
End

Evaluation of model accuracy

The prediction effect of the model was evaluated comprehensively from the aspects of accuracy and stability, and three evaluation indexes, RMSE, MAE and R^2, were selected. RMSE, MAE, and R^2 can be calculated according to Eqs. (10), (11), and (12), respectively[28]:

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}\left(y^{obs} - y^{pred}\right)^2}{n}} \tag{10}$$

$$\mathrm{MAE} = \frac{\sum_{i=1}^{n}\left|y^{obs} - y^{pred}\right|}{n} \tag{11}$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(y^{obs} - y^{pred}\right)^2}{\sum_{i=1}^{n}\left(y^{obs} - \overline{y^{obs}}\right)^2} \tag{12}$$

where y^{obs} and y^{pred} represent the observed and predicted values of the sample, respectively, $\overline{y^{obs}}$ represents the mean of the sample observations, and n represents the total number of samples.

Case study

Project context

The project is situated in a cold and saline area in the northeast region of China. Therefore, in order to solve the problem of saline-alkali corrosion, concrete must have a high resistance to chloride ion permeability. To facilitate the early-stage construction, it is necessary to optimize the concrete mix ratio, this paper obtains the test data based on the mix ratio test of expressway concrete raw materials. Chloride permeability test is shown in Figure 2. Taking C50 concrete as the object, the proposed ML algorithm predicts the CIPC of concrete effectively.

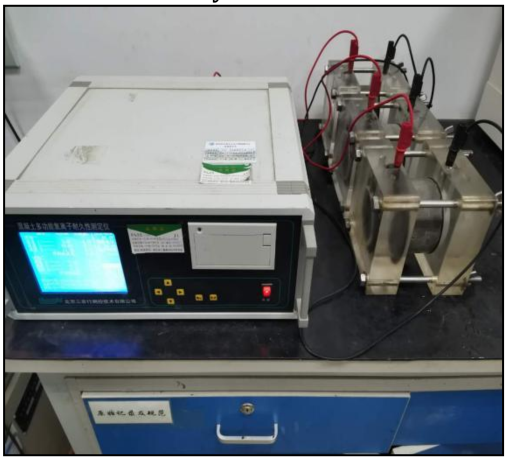


Figure 2. Chloride permeability test

Establish a sample dataset

Based on extensive literature and practical engineering experience[29], six factors including water-binder ratio (x_6), cement content(x_1), fly ash content(x_2), fine aggregate(x_4), coarse aggregate(x_3), and compound superplasticizer(x_5) have been identified to influence the CIPR of concrete. These factors are used as input variables in the construction of the primary indicator system for CIPC, with the CIPC selected as the factor variable. To conduct the study, 120 sets of orthogonal test data are obtained from actual projects. Among these, 96 sets are utilized as the training sample set, while 24 sets are allocated as the inspection sample set. The training set is utilized to determine the parameter selection for the LGBM model and build the model. The test set is then used to evaluate and validate the prediction performance of the model. Table 1 provides details of the sample data. Due to limited space, not all datasets are outlined in detail in this paper. However, the complete datasets can be obtained upon reasonable request to the corresponding authors of this paper.

Table 1. Concrete CIPR data

x_1	x_2	x_3	x_4	x_5	x_6	y
380	61	1128	685	0.9	0.34	1.35
384	57	1132	693	1.0	0.34	1.60
397	32	1117	679	0.9	0.35	1.85
...	...	...	...	...	...	...
335	59	1151	705	0.8	0.36	3.92
335	59	1151	705	1.2	0.36	3.87
335	59	1151	705	1	0.36	3.81

LGBM parameter setting

The model's parameters were adjusted to enhance the prediction accuracy of the CIPC. The search process of hyperparameter BO optimization is described in **Figure 3**, and the optimal hyperparameters with the highest prediction accuracy are shown in **Table 2**.

Table 2. Optimal hyperparameters for the highest measurement accuracy

Algorithm	Hyperparameter Selection	Optimal Hyperparameters
LGBM	colsample-bytree	0.562
	learning-rate	0.033
	minibatch_frac	0.46
	n_estimators	180

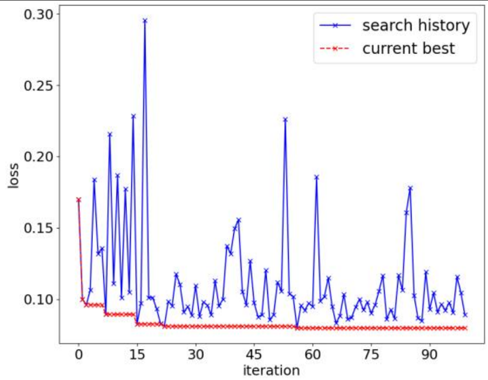


Figure 3. BO optimized hyperparameter search graph of CIPC

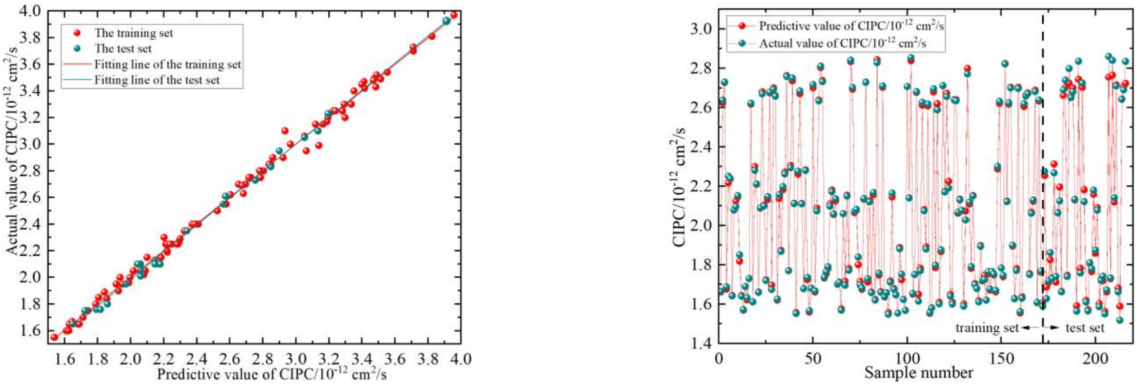
The BO algorithm has a good effect on the optimization of hyperparameters. According to the hyperparameter search graph, it can be seen that all three objectives obtain the best hyperparameters with 57 iterations, which indicates that BO optimization can search the hyperparameters effectively and find the optimal solution quickly.

Evaluation of BO-LGBM prediction results

The regression test results were obtained by optimizing LGBM parameters and modeling the training and test samples. Figure 4(a) and Figure 4(b) display the regression fitting curve for the training sample set and the prediction result of the regression fitting for the test sample set, respectively. The obtained results are as follows:

(1) The difference between the forecasted and actual values of the CIPC using LGBM is minimal. The RMSE between the real and predicted values for the CIPC in the training set is 0.045, while the RMSE in the test set is 0.098.

(2) The BO-LGBM prediction model exhibits a strong fit. The R^2 between the actual and predicted values of the CIPC in the training set is 0.974, while in the test set it is 0.955. These findings demonstrate that LGBM is a highly accurate predictor.



a. Fitting results of samples b. prediction results

Figure 4. The prediction result and prediction fitting result of CE

Discussion

Correlation analysis

In this paper, The Pearson correlation coefficient (PCC) is utilized to analyze the linear relationship between different mix proportion factors and concrete CIPR, revealing the correlation. The correlation between influencing factors and CIPR can be analyzed using the Pearson function. Figure 6 presents the PCCs between the calculated characteristic variables, displaying the correlation graph results between the variables generated by software. Blue indicates a strong positive correlation between the variables, while red indicates a negative correlation. The darkness of the square and the size of the diameter indicate the absolute value of the PCC between the two variables, reflecting the intensity of the correlation; and vice versa, the weaker the correlation degree.

Figure 6 shows that (1) The input parameters exhibit a weak correlation with no apparent coupling phenomenon. The correlation coefficient among the six parameters in Figure 6 is relatively small, indicating that there will be no obvious coupling phenomenon between the parameters, and the prediction results are reliable.(2) Lowering the water-binder ratio and reducing the amount of cement can enhance the CIPR of concrete. The correlation coefficients between the water-binder ratio and cement dosage, and the CIPC are 59% and -45%, respectively. This suggests a positive correlation between the CIPC of concrete and the water-binder ratio, a negative correlation between the CIPC of concrete and cement dosage within certain limits. Thus, in practical projects, emphasizing the reduction of the water-binder ratio can be a priority in improving the CIPR of concrete. At the same time, the amount of fly ash should be controlled.

Figure 6. The correlation between the variables

Prediction accuracy analysis

To further prove the credibility of the LGBM, SVM, BP and GBDT models are used to forecast the CIPR of concrete. For comparative analysis, the RMSE and certainty coefficient are chosen to weighs the predictive impact of the model. The aberration correlation of the prediction results of the various models is shown in Table 2.

Table 2 highlights the following findings: (1) The LGBM prediction model exhibits the lowest RMSE, closest to 0, compared to other models. In the training set, the RMSE of LGBM is 0.045, while in the test set, it is only 0.096, significantly outperforming other models. This indicates that the LGBM model yields predictions closest to the actual values and has the highest prediction accuracy. (2) The LGBM model achieves the largest R^2, closest to 1. Both in the training set and test set, the R^2 values of the LGBM prediction model are 0.967 and 0.959, respectively, surpassing the values of other models. This implies that the LGBM model provides the best fit to the data and exhibits the most accurate predictive performance. (3)The LGBM algorithm proves its adaptability and superiority in forecasting concrete CIPR. This assertion is supported by the findings of other researchers.In summary, the LGBM prediction model demonstrates superior performance in terms of accuracy, fit to the data, and prediction effectiveness for concrete CIPC. For instance, through comparing the prediction performance of five machine learning algorithms, Zhang obtained that the prediction precision of the LGBM is more excellent than that of the other algorithms [30].

Table 2 Error comparison

Model	RMSE		R^2	
	Training set	Test set	Training set	Test set
LGBM	0.045	0.098	0.974	0.955
SVM	0.41	0.322	0.888	0.882
BP	0.57	0.471	0.855	0.836
GBDT	0.087	0.224	0.922	0.911

Conclusion

To accurately and efficiently predict the CIPC of concrete, it is crucial to understand the significance of factors associated with CIPC, especially in complex and extreme environments. This study proposes an intelligent prediction model of concrete CIPC based on BO-LGBM algorithm. Using a national key project as a case study, the method's effectiveness was verified, leading to the following main conclusions:

(1) BO can effectively search and optimize the hyperparameters of LGBM. Within 100 iterations, BO optimization can search the hyperparameters effectively and find the optimal solution quickly.

(2)BO-LGBM can effectively predict CIPC of concrete. On the test set, RMSE is 0.098, R^2 is 0.955. Compared with SVM, BP and GBDT model, LGBM has higher prediction accuracy and smaller error.

(3) The BO-LGBM model can be utilized to adjust the concrete mix ratio and control the concrete quality in practical projects. The conclusion can provide guidance for intelligent prediction of other properties of concrete.

The method was successfully applied to the case project, resulting in a good CIPC of concrete. Therefore, this algorithm holds considerable potential for practical application in engineering production projects. While this study focused on the principles influencing the CIPC at the concrete material mix proportion level, it is worth noting that concrete curing measures also play a role in the CIPC. Moving forward, it is important to consider additional factors.

Data Availability Statement

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

Acknowledgement

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Nomenclature

BO	Bayesian Optimization
GS	Grid search
RS	Random search
LGBM	Light Gradient Boosting Machine
-	Cement(x_1), kg/m^3
-	Fly ash(x_2), kg/m^3
-	coarse aggregate(x_3), kg/m^3
-	fine aggregate(x_4), kg/m^3
-	water-binder ratio(x_5)
-	compound superplasticizer(x_6),%
CIPC	Chloride ion permeability coefficient(y), 10^{-12} cm^2/s
CIPR	Chloride ion penetration resistance

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