

Prediction of Calcined Coke Powder Resistivity Based on XGBoost

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Abstract

This paper addresses the quality prediction in the carbon calcination process by collecting operational data from a rotary kiln control system and material assay analysis data for 7 months, which were pre-processed to set up a time-series feature data set. The SelectKBest method was used for feature dimensionality reduction in the study to select key influencing factors such as calcination temperature, revolution speed of rotary kiln, and kiln head negative pressure. Based on these factors, a gradient boosting decision tree (XGBoost) prediction model for powder specific resistivity was set up, with its structure and parameters automatically optimized via GridSearchCV. This model was compared with traditional algorithms like Support Vector Machine (SVM) and Backpropagation (BP) neural networks, in which the results show that the XGBoost model achieved the best performance, with a coefficient of determination $R^2 > 0.91$ on the test set. The study indicates that the prediction model can effectively capture the non-linear relationships in the carbon calcination process by combining feature engineering and the XGBoost algorithm, which enables timely prediction of calcined coke powder specific resistivity to provide reliable predictive support for quality optimization in the production process and hold practical significance for advancing the intellectualization of the calcination process.

Keywords: Calcined coke, Powder specific resistivity, XGBoost, Prediction model.

1. Introduction

As a core raw material for prebaked anode production, the powder resistivity of calcined coke is a key indicator that determines the conductive performance of anodes used in aluminium electrolysis, directly correlating with the current efficiency and energy consumption level of the aluminium electrolysis process. Therefore, indicator prediction in the calcination process holds significant practical importance for optimizing production decisions in advance and promoting energy saving in the carbon calcination process. However, the powder specific resistivity of calcined coke is affected by multiple factors including the properties of petroleum coke raw material, calcination temperature, and soaking time in a coupling manner to exhibit complex non-linear relationships [1]. Traditional resistivity measurement relies on offline laboratory assays, which suffer from long testing cycles and serious hysteresis, making it difficult to reflect production dynamics in a timely manner and thus restricting the refined control of the carbon calcination process.

Recently, machine learning technology has been widely applied in industrial scenarios such as key indicator prediction and fault diagnosis due to its powerful non-linear modelling capabilities and efficient data processing characteristics [2–5]. Among these technologies, XGBoost is an ensemble learning algorithm that has demonstrated excellent performance in multiple domains

due to its advantages in both prediction accuracy and computational efficiency. Combined with the ARIMA model, Chen Fei et al. [6] used XGBoost to predict lithium battery SOC, improving indicators like absolute error and root mean square error by 15–20 % through a residual correction strategy; Linkai Sun et al. [7] used XGBoost to classify faults in test bench monitoring data, and by incorporating data augmentation techniques such as Gaussian noise addition and feature rotation, the classification accuracy has been increased up to 98.1 %, fully verifying its applicability in complex industrial scenarios.

In carbon production, the application of machine learning methods also becomes increasingly popular. Yujie Zhao et al. [8] proposed an XLG-BP fusion algorithm for predicting the powder specific resistivity of calcined coke and developed a corresponding online prediction system to significantly improve the response speed of the algorithm and prediction accuracy; Wuqun Wang [9] used CART decision tree and random forest algorithms to predict four key physical and chemical indicators of calcined petroleum coke to achieve an overall accuracy of 92 %, which provided a new approach for quality control in carbon production.

To address the demand for predicting the resistivity of calcined coke, this study develops an XGBoost prediction model based on process control data and material assay parameters from the carbon calcination process, which incorporates feature dimensionality reduction via the SelectKBest methodology to identify key influencing factors, followed by hyperparameter optimization using GridSearchCV and validation against traditional algorithms like SVM and BP neural networks, thereby delivering a high-precision predictive tool for advancing quality optimization and the intelligent upgrading of the carbon calcination process.

2. Related Theories and Methodology

2.1 XGBoost Algorithm

The XGBoost algorithm uses the Boosting Tree as its core framework, of which the central idea is to iteratively generate a series of weak classifiers (CART trees) that are combined into a strong classifier through a weighted ensemble, introducing an approach known for its high accuracy, computational efficiency, and capability in handling high-dimensional data. As shown in Equation (1), the objective function of this algorithm consists of two core components, which are a loss function that measures the difference between the predicted and true values, and a regularization term (e.g., tree depth, number of leaf nodes) that incorporates node weights to control model complexity and effectively mitigate over fitting.

$$L(\theta) = \sum_{i=1}^{\infty} l(y_i, y'_i) + \sum_{k=1}^{\infty} \Omega(f_k) \quad (1)$$

where:

$l(y_i, y'_i)$ Loss between the predicted value y'_i and the true value y_i for the i -th sample
 $\Omega(f_k)$ Regularization term of the k -th tree model

2.2 SelectKBest Feature Dimensionality Reduction

SelectKBest is a filter-based feature selection method. Its core principle is to quantify the correlation strength between each feature and the target variable through statistical tests, thus selecting the k features with the strongest correlation. The resulting feature subset reduces data dimensionality while retaining key information, laying the foundation for efficient input in subsequent model training.

(1) Feature scoring: Each feature X_i is evaluated independently to calculate its statistical

correlation score with the target variable (including the F value and its corresponding p value). This process considers no mutual dependence between features. The scoring results depend on the scoring function having been adopted, as different functions correspond to different logic of statistical testing and calculation methods. Commonly used functions include F-test, chi-squared test, ANOVA F-test, and mutual information. This paper adopts the F-test as the scoring function for the regression task, generating scores by quantifying the linear correlation between features and the target variable, as detailed in Equation (2).

(2) Feature selection: Based on the feature scoring, the features are sorted in descending order, in which the top k features with the highest scores are selected to form a concise feature set, thus achieving effective data dimensionality compression.

$$F = \frac{\text{Between group variance}}{\text{Within group variance}} = \frac{MS_{model}}{MS_{error}} \quad (2)$$

where:

MS_{mode} Mean square of the model, representing explainable variance

MS_{error} Mean square error of the residuals, representing the unexplained variance

2.3 GridSearchCV Parameter Optimization

GridSearchCV is a classic tool in the scikit-learn library for hyperparameter optimization. Its core mechanism is to combine Grid Search with Cross-Validation (CV) to systematically search for optimal hyperparameter configuration, avoiding subjectivity in hyperparameter tuning. It can reliably obtain parameter configurations that are well adapted to the data set, particularly suitable for fine-grained optimization in small to medium-sized parameter spaces. Including:

(1) Hyperparameter grid construction: For the target model, a set of candidate values for each hyperparameter is predefined to form a multi-dimensional parameter grid, enumerating all possible hyperparameter combinations.

(2) Cross-validation evaluation: The training set is divided into k folds (typically k=5 or 10). For each hyperparameter combination, cross-validation is done through iterative cycles of "training on k-1 fold and validating on 1 fold", and the average performance indicator from the k validations is calculated as the evaluation score for that combination.

(3) Optimal parameter selection: The average cross-validation scores of all hyperparameter combinations are compared, in which the combination with the highest score is selected as the optimal hyperparameter configuration θ^* .

(4) Final model training: Based on the optimal hyperparameters θ^* , the model is retrained on the entire training set and its generalization performance is evaluated on an independent test set to ensure the reliability of the parameter optimization.

2.4 Model Evaluation Indicators

Three commonly used evaluation indicators in regression tasks are determination coefficient (R^2), mean relative error (MRE), and mean squared error (MSE). The lower the values of these 3 indicators, the higher the prediction accuracy of the model. R^2 presents how much of the variance of the label variables in the regression model can be explained by the feature variables, with a value ranging from 0 to 1. A higher R^2 value signifies a better fit of the model to the data; MRE reflects the degree of relative deviation between the predicted and true values; MSE measures the average size of the squared prediction errors and is more sensitive to larger errors, thus

highlighting the impact of extreme deviations.

$$R^2 = 1 - \frac{\sum_{i=0}^n (y_i - y'_i)^2}{\sum_{i=0}^n (y_i - \bar{y})^2} \quad (3)$$

$$\text{MRE} = \frac{1}{n} \sum_{i=1}^n \frac{|y_i - y'_i|}{|y_i|} \quad (4)$$

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^n (y_i - y'_i)^2 \quad (5)$$

where:

- n Number of samples
- y_i True value of the samples
- \bar{y} Mean value of samples
- y'_i Predicted value of samples

3. Experiment Design and Data Processing

3.1 Experimental Data

This paper collected historical production data from the carbon calcination process of a certain carbon enterprise, covering 7 months of operational data from the rotary kiln control system and assay analysis data for calcined coke from January to July 2023. The rotary kiln control system data were collected at 2-minute intervals, including 31 feature parameters primarily involved in process parameters and equipment status indicators, which are petroleum coke feed rate, calcined coke output, kiln head temperature, calcination temperature, dust settling chamber inlet and outlet temperatures, kiln tail temperature, discharge temperature, exhaust temperature, downcomer temperature, negative pressure in the kiln head and dust settling chamber, rotary kiln motor speed, secondary and tertiary air fan speeds, and material levels in the pre-calcination silo and calcined coke silo; The label data is the calcined coke powder specific resistivity (unit: $\mu\Omega \cdot m$), collected at 4-hour intervals. The original distribution characteristics of the feature data are detailed in Table 1.

3.2 Data Pre-processing

To reconcile the temporal discrepancy between the feature data (2-minute intervals of fine grain size) and the label data (i.e., the calcined coke powder specific resistivity at 4-hour intervals of coarse grain size), a pre-processing methodology was developed that integrates time grain size alignment and lagged feature fusion. This approach yielded a data set of over 600 valid samples and 156 time-series features, in which each sample comprises current features, lagged features from the preceding four hours, and the resistivity value from the previous time step, thereby effectively capturing the dynamic characteristics of the rotary kiln calcination process and laying a solid foundation for the subsequent construction of a high-precision prediction model.

Table 1. Statistical characteristics of feature parameters in calcination process.

Parameters	Units	Mean	Standard deviation	Minimum	Median	Maximum
Set feed rate of petroleum coke	t/h	7.87	0.68	0.00	8.00	9.50
Instantaneous output of calcined coke	t/h	6.37	1.98	0.00	6.29	10.00
Kiln head temperature	°C	844.1	37.7	611.4	844.4	1053.8
Calcination temperature	°C	1233.9	43.3	700.0	1236.9	1325.7
Inlet temperature of dust settling chamber	°C	1034.1	64.3	404.7	1044.2	1156.6
Outlet temperature of dust settling chamber	°C	1119.9	82.2	436.3	1141.2	1290.6
Exhaust temperature	°C	153.78	15.46	18.40	152.78	245.57
Discharge temperature	°C	77.68	15.39	12.07	76.48	166.23
Downcomer temperature	°C	32.82	4.69	19.44	32.64	54.51
Desulfurization flue gas flow rate	Nm ³ /h	56 149	10 817	0.00	57 698	79 878
Kiln head negative pressure	Pa	-0.16	4.08	-26.48	0.17	16.41
Inlet negative pressure of dust settling chamber	Pa	-56.79	12.66	-93.66	-56.77	-2.60
Outlet negative pressure of dust settling chamber	Pa	-72.63	13.59	-114.2	-72.74	-15.28
Desulfurization blower frequency	Hz	39.49	5.46	0.00	39.99	48.99
Air inlet opening of dust settling chamber	%	20.94	24.52	0.00	3.96	100.00
Exhaust blower speed	r/min (Hz)	46.73	3.29	0.16	47.41	49.68
Secondary air motor speed	r/min	2279.3	251.7	0.0	2350.0	2502.0
Tertiary air motor speed	r/min	1288.6	169.7	0.0	1301.0	1778.0
Rotary kiln motor speed	r/min	847.34	64.98	0.00	852.00	910.00
Furnace front temperature	°C	809.48	77.58	81.94	812.15	963.89
Furnace rear temperature	°C	341.60	26.27	72.19	344.62	390.63
Furnace front negative pressure	Pa	-147.8	23.21	-16.1	-149.3	-24.0
Furnace rear negative pressure	Pa	-179.9	29.86	-265.5	-182.6	-25.3
Boiler water level	mm	58.51	26.13	-49.14	57.67	186.01
Steam pressure	Mpa	0.76	0.07	0.02	0.77	0.91
Deaerator water temperature	°C	84.93	38.86	0.00	102.60	105.90
Pre-calcination silo level	m	5.92	0.88	2.88	5.88	7.71
No. 1 Calcined coke silo level	m	10.04	4.89	0.28	9.87	20.63
No. 2 Calcined coke silo level	m	12.42	5.92	2.82	11.30	19.47
Superheater inlet steam temperature	°C	153.16	6.51	28.79	153.65	198.78
Superheater outlet steam temperature	°C	223.53	14.17	30.67	224.54	262.01

(1) Fine grain size data pre-processing

First, data cleaning was performed on the original 2-minute interval feature data, including 0 value detection, null value removal, and outlier removal (based on the 3σ criterion). Then, the max-min normalization method was used for standardization to eliminate the influence of different scales among features. Figure 1 shows an example of the calcination temperature parameter, where the removal of abnormal data points that fall outside the 3σ criterion, specifically data points below the process lower limit of $1100\text{ }^{\circ}\text{C}$, to make the data distribution more consistent with actual carbon production conditions.

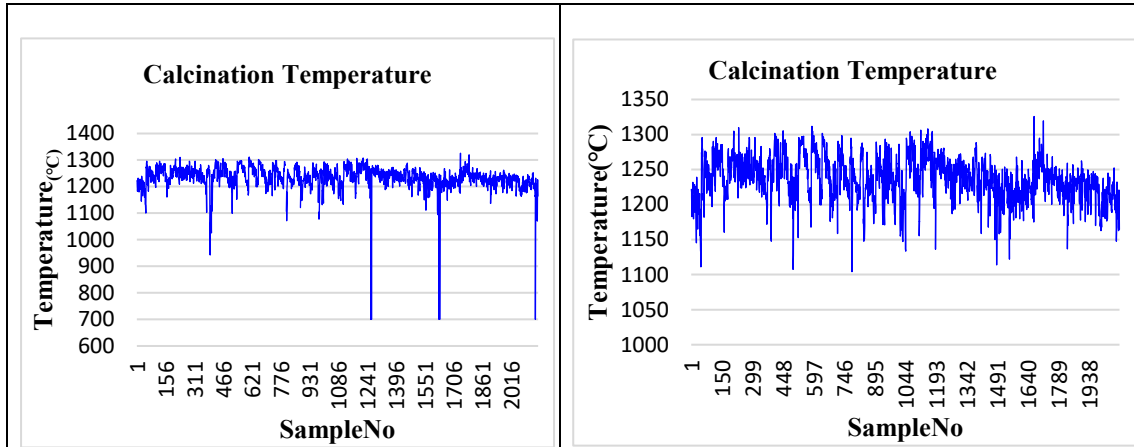


Figure 1. Some 2-minute data of calcination temperature. left: before pre-processing, right: after pre-processing.

(2) Multi-scale time grain size alignment

Feature down-sampling was performed on the pre-processed fine grain size data, extracting the first record of each hour to construct an hourly feature sequence. Given the slow variation of rotary kiln process parameters and their lagged impact on quality indicators, lagged features from the previous 4 hours (X_{t-1} , X_{t-2} , X_{t-3} , X_{t-4}) and the resistivity label from the previous time step (Y_{t-1}) were specifically constructed. By using a sliding window technique, the hourly features were matched with the 4-hour interval resistivity labels to form a complete time-series mapping relationship.

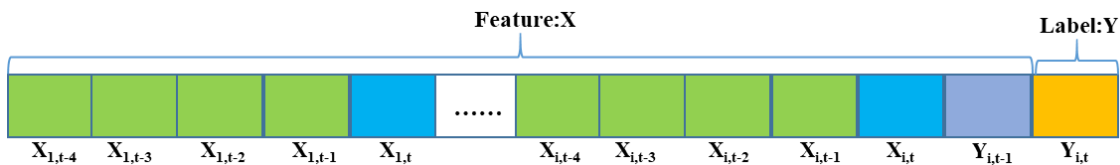


Figure 2. Schematic diagram of calcination time series data set.

3.3 Prediction Model Establishment

The data analysis and model development in this study were conducted in a unified hardware and software environment: Ubuntu 22.04 as the OS, Python 3.12 as the programming tool, and the algorithm deployment based on the PyTorch framework; The hardware configuration included Intel i9-13900K processor, NVIDIA GeForce RTX 4090 D graphics card (24 GB VRAM), and 64 GB of memory, providing stable computational support for large-scale data processing and complex model training.

The framework of the calcined coke powder specific resistivity prediction model, based on SelectKBest feature selection and the XGBoost algorithm, is shown in Figure 3 and mainly includes:

- (1) Data pre-processing: Collect real-time operational data from the rotary kiln control system and assay data of calcined coke powder specific resistivity from the calcination process; improve data quality through pre-processing steps such as data cleaning, outlier handling, and missing value imputation; use the SelectKBest method to select key features that are closely correlated with the target variable.
- (2) Model building: Input the selected feature data into the XGBoost model. By building an objective function centered on a loss function and a regularization term, the prediction problem is transformed into a function minimization problem, in which the model parameters are continuously optimized through an iterative learning mechanism to enhance overall prediction performance.
- (3) Hyperparameter optimization: Use the GridSearchCV method to find the optimal hyperparameters for the XGBoost model. Evaluate the performance of different parameter combinations through cross-validation and select the best configuration to further improve prediction accuracy and reduce prediction error.
- (4) Model evaluation: Divide the data into training and test sets for model training and prediction. Analyze the performance of the model based on the predefined evaluation indicators of MSE, MRE, and R^2 to validate the effectiveness of the proposed method.

The modelling data set was obtained by performing parameter optimization on the pre-processed time series data set using SelectKBest. The parameters for SelectKBest include the number of features to retain and the scoring function. The number of features to be retained (k) was grid-searched over range (3, 156, 5), i.e., from 3 to 156 with a step of 5; The scoring function (score_func) selected was f_regression, which is suitable for regression tasks.

The modelling data set was divided chronologically into a 4:1:1 ratio, with the first 400 samples (January to April) as the training set, the next 100 samples (May to mid-June) as the validation set, and the final 100 samples (mid-June to July) as the test set. On the same training and test sets, powder specific resistivity prediction models were constructed by using SVM, BP neural network, and XGBoost, respectively. The parameter ranges for each model were set as follows:

- (1) SVM parameters included the kernel coefficient, insensitivity zone width, kernel function parameters, and kernel function type. The kernel function types included ['linear', 'rbf', 'poly'], kernel coefficients included [0.1, 1, 10, 100], the insensitivity zone width included [0.01, 0.1, 0.2], and kernel function parameters included ['scale', 'auto', 0.1, 1].
- (2) BP parameters included the learning rate, number of iterations, optimizer, and loss function. The learning rate included [0.001, 0.01, 0.1, 0.2, 0.5], the number of iterations was set to 500, the optimizer was Adam, and the loss function was mean squared error.
- (3) XGBoost parameters included the number of trees, learning rate, maximum depth of tree, sum of min. child weights, sub-sampling ratio, feature sampling ratio, L1 regularization coefficient, and L2 regularization coefficient. Number of trees (n_estimators), search range (50, 500, 10), from 50 to 500, with a step of 10; Learning rate (learning_rate): [0.01, 0.1, 0.2, 0.5, 0.8]; Max. depth of tree (max_depth): range (2, 20, 1); Sum of min. child sample weights (min_child_weight): range (1, 10, 1); Sub-sampling ratio (subsample): [0.5, 0.7, 0.8, 1.0]; Feature sampling ratio (colsample_bytree): [0.5, 0.6, 0.7, 0.8]; L1 regularization coefficient (reg_alpha): [0.1, 0.2, 0.5,

0.7]; L2 regularization coefficient (reg_lambda): range (1, 10, 1).

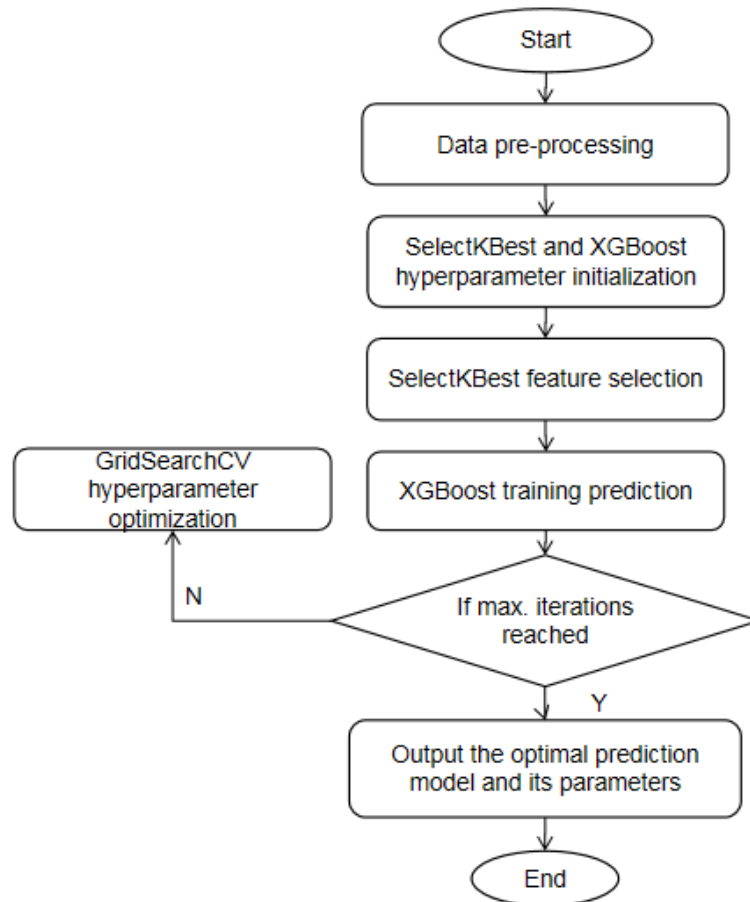


Figure 3. Overall framework of powder specific resistivity prediction model.

4. Experimental Results and Analysis

4.1 Feature Dimensionality Reduction

The feature selection results are shown in Figure 4. The model's mean squared error (MSE) reached its minimum when $k=78$. The key features selected at this point are shown in Figure 5, including calcination temperature, exhaust temperature, desulfurization blower frequency, superheater inlet steam temperature, desulfurization flue gas flow rate, discharge temperature, rotary kiln motor speed, furnace front negative pressure, kiln head negative pressure, and the powder specific resistivity at time $t-1$. The feature importance scores for the powder specific resistivity at time $t-1$, kiln head negative pressure, and superheater outlet steam temperature all exceeded 5.

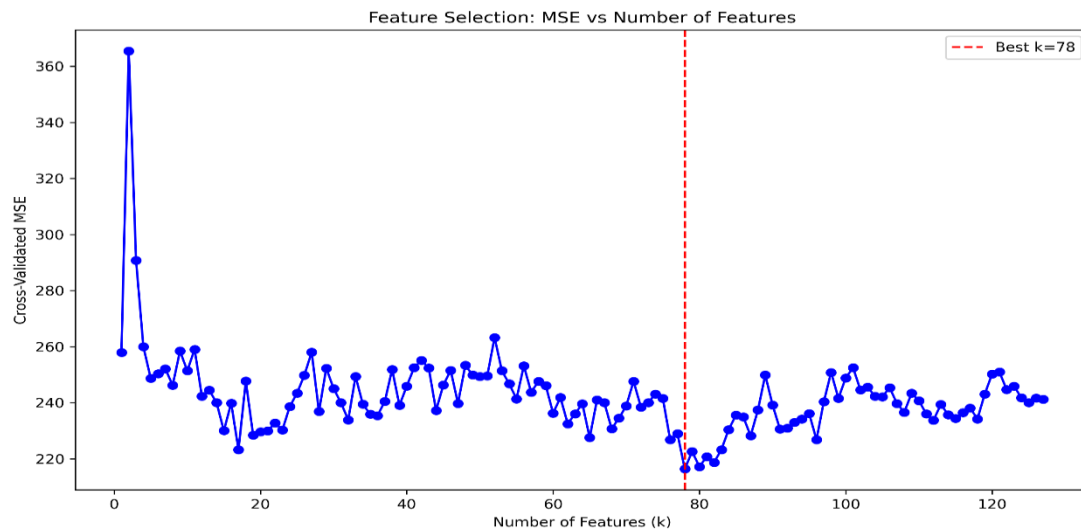


Figure 4. MSE under different k values for SelectKBest.

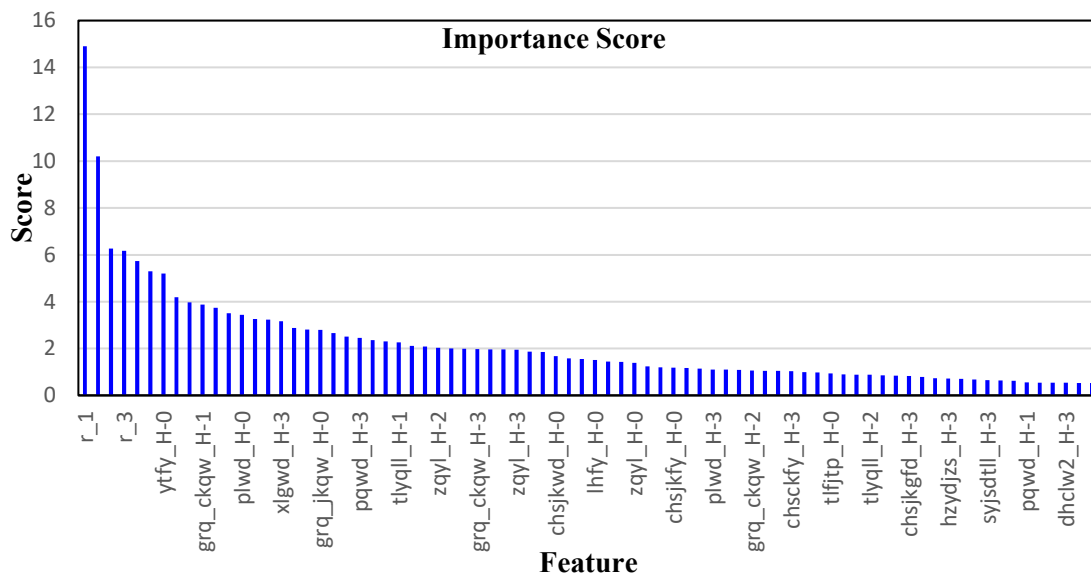


Figure 5. Feature importance scores.

4.2 XGBoost Parameter Optimization Results

Five-fold cross-validation and GridSearchCV were used for automatic hyperparameter tuning, with the determined optimal parameters shown in Table 2. Among these parameters, $n_estimators = 300$, $learning_rate = 0.1$, $max_depth = 5$, and $reg_lambda = 5$.

4.3 Model Prediction Performance

After model training, the best-performing model was selected to predict the 100 sample groups in the test set. The results are shown in Figure 6. In the figure, the horizontal axis represents the sample index of the test set, and the vertical axis represents the calcined coke powder specific resistivity, the blue curve represents the true values, and the orange curve represents the values

predicted by the model. The visualization results show that the predicted values closely follow the trend of the true values, demonstrating a dynamic capability to capture process fluctuations. The performance indicators of the XGBoost model on the test set include coefficient of determination R^2 which reached 0.914, indicating that the model can explain 91.4 % of the target variable's variance; the mean squared error (MSE) was 42.01 $\mu\Omega\cdot m$, and the mean relative error (MRE) was 3.1 %, approximately 90 % of the sample prediction errors were concentrated within the ± 3 % range, validating the model's reliability in actual production scenarios.

Table 2. XGBoost hyperparameter ranges.

Hyperparameter	Hyperparameter description	Hyperparameter range	Optimal hyperparameter
max_depth	Max. depth of tree	range(2, 20, 1)	5
learning_rate	Learning rate	[0.01, 0.1, 0.2, 0.3]	0.1
n_estimators	Number of trees	range(50, 500,10)	300
min_child_weight	Sum of min. sample weights required by child nodes	range(1, 10, 1)	3
gamma	Min. loss reduction required for node splitting	range(0.1, 5, 0.5)	0.8
subsample	Subsample ratio	[0.5, 0.7, 0.8, 1.0]	1
colsample_bytree	Construct sampling ratios for each tree's time-series feature	[0.5, 0.6, 0.7, 0.8]	0.6
alpha	L1 regularization	[0.1, 0.2, 0.5, 0.7]	0.1
Lamda	L2 regularization	range(1, 10, 1)	5

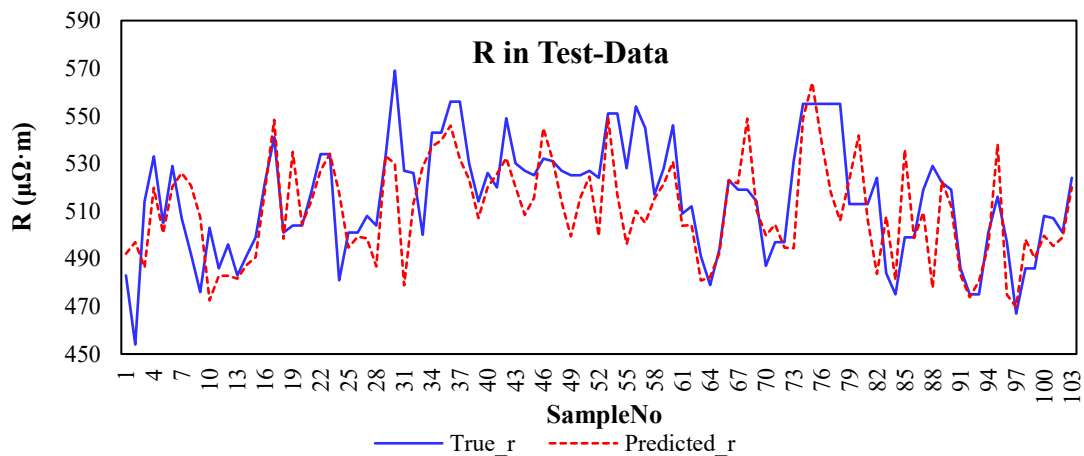


Figure 6. Prediction effect of XGBoost model on test set.

Table 3 lists the performance indicators (R^2 , MSE, MRE) of the three models (SVM, BP neural network, and XGBoost) on the test set. The results show that the coefficient of determination R^2 for all three models was greater than 0.83, indicating that all possess good predictive capabilities. In particular, the XGBoost model performed the best, with an R^2 of 0.91 and a mean relative error of 3 %.

Compared to SVM, XGBoost's mean squared error (MSE) was reduced by 32 %, and its mean relative error (MRE) was reduced by 4.7 %; compared to the BP neural network, XGBoost's MSE

was reduced by 16 %, and its MRE was reduced by 1.9 %. The above results indicate that the XGBoost model outperforms the compared models in both error control and prediction accuracy, with a particularly prominent advantage in reducing MSE, thereby validating its applicability for quality prediction in the carbon calcination process.

Table 3. Performance indicators of prediction models.

Modeling Approach	R ²	MSE	MRE (%)
SVM	0.847	74.642	7.872
BP Neural Network	0.881	58.033	5.059
XGBoost	0.914	42.007	3.155

5. Conclusion

This paper collected real-time operational data from a rotary kiln control system and assay analysis data of calcined coke from January to July 2023. By pre-processing steps including time grain size alignment, outlier removal, and feature standardization, a time series data set with over 600 valid samples was constructed. The SelectKBest feature selection method was used for dimensionality reduction to select key features that significantly affect the powder specific resistivity of calcined coke, laying a high-quality data foundation for model construction.

Based on the pre-processed data set, three prediction models (SVM, BP neural network, and XGBoost) were constructed, and the hyperparameters for XGBoost were automatically optimized using GridSearchCV. Comparative experiments indicated that the XGBoost model performed the best, achieving a coefficient of determination R² of 0.91 on the test set with the mean relative error controlled within 3 %. Its MSE was 32 % lower than the SVM model's and 16 % lower than the BP neural network's, validating its capability to capture non-linear process relationships.

This study indicates that a prediction model built on industrial process data and machine learning algorithms can achieve accurate prediction of calcined coke powder specific resistivity, providing reliable model support for the intelligent control of the carbon calcination process.

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