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.

$$\mathrm{L}(\emptyset) = \sum_{i=1}^{\infty} l(y_i, y_i') + \sum_{i=1}^{\infty} \Omega(f_k) \tag{1}$$

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

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 R^2 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.

6. References

1. Hao Li, et al., The Influencing Factors and Improvement Measures of Calcined Coke Quality in Pot Calciner, *Light Metals*, 2011, (3), 43–46 (in Chinese).
2. Jinghui Niu, Key Data Prediction Algorithm for Industrial Wastewater Quality Based on GWO-XG Boost, *Industrial Water Treatment*, 2024, 44(1), 184–190 (in Chinese).
3. Peng Zhao, Wenjian Wang, et al., Anomaly Detection in Blockchain Based on XGBoost and Random Forest, *Journal of Nanjing University of Posts and Telecommunications (natural Science Edition)*, 2025, 45(1), 115–122 (in Chinese).
4. Yi Zeng, *Research on Energy Demand Forecasting Based on BP Neural Network Optimized by Differential Evolution Algorithm*, Master's thesis, Huazhong University of Science and Technology, 2015 (in Chinese).
5. Linkai Sun, Kang Lou, Fault Diagnosis of Controllable Pitch Propeller Hydraulic System Test Bench Based on XGBoost Method, *Ship Engineering*, 2024, 46(S2), 190-196 (in Chinese).
6. Manshan Lin, Ziyu Liu, *Quality Analysis and Research on Anode Calcination Process Parameters*, *Software*, 2019, 40(7), 166–168 (in Chinese).
7. Chen Fei, Shuxiang Song, et al., Soc Estimation of Lithium-Ion Battery Based on XGBoost Prediction and Arima Residual Correction, *Journal of Wuhan University of Technology*, 2019, 41(10), 94–101 (in Chinese).

8. Yujie Zhao, *Research and Application of Prediction Algorithm for Powder Resistivity of Anode Calcined Coke*, Master's thesis, North China University of Technology, 2022 (in Chinese).
9. Wuqun Wang, *Research and Analysis of Calcination Process Parameters Based on Decision Tree*, Master's thesis, North China University of Technology, 2018 (in Chinese).