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Operating Key Factor Analysis of a Rotary Kiln Using a Predictive Model and Shapley Additive Explanations

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Abstract: The global smelting business of nickel using rotary kilns and electric furnaces is expanding due to the growth of the secondary battery market. Efficient operation of electric furnaces requires consistent calcine temperature in rotary kilns. Direct measurement of calcine temperature in rotary kilns presents challenges due to inaccuracies and operational limitations, and while AI predictions are feasible, reliance on them without understanding influencing factors is risky. To address this challenge, various algorithms including XGBoost, LightGBM, CatBoost, and GRU were employed for calcine temperature prediction, with CatBoost achieving the best performance in terms of MAPE and MLSE. The influential factors on calcine temperature were identified using SHAP from XAI in the context of the CatBoost model. SHAP effectively assesses model impacts, accounting for variable interdependencies, and offers visualization in high-dimensional contexts. Given the correlation and dimensionality of variables predicting calcine temperature, SHAP was preferred over Feature Importance or PDP for the analysis. By incorporating seven out of twenty operational factors like burner fuel and reductant feed rate, combustion conditions inside of the rotary kiln and RPM, the calcine temperature increased from 840 °C in 2023 to 910 °C by October 2024, concurrently reducing the electricity unit consumption of the electric furnace by 7.8%. Enhancements to the CatBoost algorithm will enable the provision of guidance values after optimizing key variables. It is expected that managing the rotary kiln's calcine temperature according to the predictive model's guidance values will allow for autonomous operation of the rotary kiln through inputting guidance values to the PLC.

Keywords: pyrometallurgy; rotary kiln; CatBoost; XAI; SHAP

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1. Introduction

The objective of this study is to identify the deviation between the actual calcine temperature of rotary kilns involved in ferronickel production and the predicted values generated by machine learning and deep learning models. Additionally, the study aims to identify key variables influencing the predictions using XAI's Shapley Value Explanations. Subsequently, the goal is to reduce the calcine temperature deviation at a targeted temperature by utilizing these key variables. A rotary kiln, utilized as a rotating furnace, utilizes a burner to provide a heat source for heating and processing raw materials while rotating a structure made of refractory material that can endure high temperatures within a lengthy steel cylinder [1]. In recent times, investments in rotary kilns using the rotary kiln and electric furnace (RK-EF) method for producing nickel, a primary material for secondary batteries, have been actively progressing in nations like Indonesia [2]. In the RK-EF process, a rotary kiln serves as a preliminary reduction process to create calcine, which is sintered nickel ore, for feeding to an electric furnace. The raw materials include nickel ore and a reductant, with a fuel like pulverized coal or LNG being injected into a burner to act as a heat source for burning the reductant. Nickel ore is initially supplied with around 20~35% moisture content, and as the adhering moisture is dried, the crystalized moisture is

eliminated, following which it is discharged from the rotary kiln, reaching temperatures of approximately 700~1050 °C. Raw materials such as ore are natural resources, exhibiting significant variations in composition and particle size [3]. For instance, smelters producing ferronickel utilize a blend of ore with nickel content ranging from 1.4 to 2.6% and iron content between 9 and 25%. The reaction occurring in the rotary kiln alters with changes in the iron content of the ore, necessitating adjustments to the operational settings of the rotary kiln, depending on the dust production rate [4]. The raw materials utilized in rotary kilns, such as ore and coal, are sourced from nature, and variations in composition and particle size can impact rotary kiln operations [5]. Additionally, issues like malfunctions in front- and rear-end equipment, like clinker formation which comes from overheating and dust-generation rate increase, can alter the calcine quality and productivity of the rotary kiln.

Calcine is produced roughly ninety minutes after the ore is introduced into the rotary kiln and then discharged from the kiln. To ensure the effective and economical functioning of the electric furnace process downstream of the rotary kiln, enhancing the calcine temperature is imperative, along with minimizing temperature deviations [6]. Various factors can influence the calcine temperature of a kiln, such as the quantity of ore, pellet, coal for reduction, coal through the scoop feeder, and amounts of pulverized coal to the burner, pressure in the rotary kiln, concentrations of CO(g), O_2(g), SOx, NOx in the offgas, and the temperature of the kiln body. Therefore, identifying the key variables that influence the calcine temperature and analyzing operational factors, such as coal-feed-rate and air ratio, which can determine operational adjustments in response to changes, are essential for precise control of the calcine temperature in the rotary kiln [7].

A common method to measure calcine temperature involves utilizing a thermocouple [8]. Given that only around 6 to 8% of the internal volume of a rotary kiln comprises calcine, continuous temperature monitoring is challenging, even with two thermocouples positioned at 180-degree intervals. The temperature of the calcine under measurement is directly influenced by the burner flame temperature, as well as the flow rate and pressure of the primary- and secondary-combustion air supplied to the kiln burner [9]. Moreover, thermocouples placed in high-temperature zones have a relatively short lifespan of a few months, due to oxidation in high-temperature environments and abrasion from ore, even when shielded in a protective tube [10]. Alternatively, non-contact temperature measurement devices like pyrometers that detect infrared radiation energy emitted by calcines can be employed, yet they face limitations in addressing issues related to significant errors in measured values linked to the extent of dust generation [11].

Numerous scholars have analyzed sintering conditions by examining flame images [12]. Raw materials within rotary kilns undergo sintering when they surpass a specific temperature, and the calcine temperature serves as an indicator for identifying sintering conditions [13]. However, flame images are subject to various influencing factors, including dust generation due to raw-material characteristics, burner primary- and secondary-combustion air flow rates and pressures, as well as the quantity and quality of fuel supplied to the burner [14]. The utilization of flame images for measuring sintering conditions is constrained due to alterations in flame brightness and shape resulting from the mentioned factors [15]. Furthermore, research based on flame images is limited in deducing the factors influencing the control of calcine temperature to a predicted level by distinguishing and anticipating sintering conditions, such as overheating, normal sintering, and undercooling [16].

When it comes to the design of a rotary kiln, the initial step involves conducting mass-balance and heat-balance calculations. The heat produced by the burner through the combustion of coal injected with the raw material is used to generate heat, which is then discharged as sensible heat of calcine, shell heat loss of the rotary kiln body, and exhaust gas. This heat is utilized to dry the moisture present in the raw material and alter the phase of the raw material. An assessment based on heat balance can be carried out to estimate the temperature of calcine using available data. However, such an evaluation necessitates

the expertise of an individual with practical knowledge of the rotary kiln process [17]. The raw materials fed into the rotary kiln are transformed into calcine after a few hours. Since the heat supplied by the burner is released as exhaust gas after interacting with the raw material within a few seconds, it is essential to consider time delays [18]. Consequently, forecasting the temperature of calcine through induction modeling and simulation, as well as predicting calcine temperature based on mass and heat balance, is limited due to low accuracy levels, because the internal condition of the rotary kiln varies in time, not in equilibrium, all the time [19].

To address these limitations, researchers have predicted calcine temperature by modeling based on the analysis of extensive operational data. Firstly, fuzzy rules serve as an efficient method for managing uncertain and ambiguous information by simulating human reasoning processes. Nevertheless, interpreting the outcomes requires the expertise of individuals experienced in establishing numerous rules [20]. Secondly, the Support Vector Machine (SVM) can optimize margins even with limited data, ensuring a well-suited model and reducing overfitting [21]. However, the process of converting time-series data into a format for SVM modeling and feature extraction is complex. Since SVM is a black box model, it may pose challenges in identifying factors influencing model predictions and explaining results [22]. Moreover, SVM heavily relies on hyperparameters, leading to additional computational costs to determine optimal settings [23]. Thirdly, Recurrent Neural Networks (RNNs) like Long Short-Term Memory (LSTM) necessitate substantial data and are prone to overfitting [24]. Although they excel in nonlinear and time-delay studies, predictive calculations are time-consuming, especially during remodeling [25].

Recent investigations concerning the prediction of temperatures within rotary kilns have utilized methodologies such as genetic algorithm-optimized random forest (GA-RF) [26], temporal convolutional network (TCN) augmented by a long short-term memory (LSTM) architecture [27], dual-stage attention sequence-to-sequence (DA-Seq2Seq) algorithm [28], and a generative adversarial network (GAN) based on global recurrence plot (GRP) combined with long short-term memory (LSTM) [29], referred to as GRP-lstmGAN, as well as nonlinear autoregressive neural network (NARX) models [30]. In terms of performance, GRP-lstmGAN and DA-Seq2Seq excel at capturing complex patterns, offering outstanding predictive performance, but at the cost of high computational resources and training time. As an aspect of simplicity and speed, GA-RF or NARX are more appropriate, as they require fewer resources and less training time. For interpretability, the Dual-Stage Attention Seq2Seq model offers a strong balance between predictive power and model transparency, making it a good choice where understanding model decisions is critical. This analysis is constrained by the fact that the predictive outcomes were obtained from studies aimed at enhancing the forecasting efficacy of temperature predictions in rotary kilns through the integration of multiple algorithms; consequently, it fails to furnish insights regarding the critical determinants influencing calcine temperature [31], thereby limiting the operators' ability to exercise control over calcine temperature effectively. The focus should be on identifying the influencing variable rather than predicting a precise value. Recognizing the key operational factor allows for targeted controls and management, facilitating the development of a guidance model via future optimization methods.

Explainable Artificial Intelligence (XAI) emerges as a solution to this challenge [32]. This study aims to elucidate the factors influencing calcine temperature by quantitatively predicting their contribution to model predictions using SHAP (SHapley Additive exPlanation) techniques of XAI. SHAP boasts game theory attributes that ensure a fair distribution of Shapley values, enabling intuitive and equitable calculation of predictive contributions. Being model-agnostic, SHAP can be applied across various machine learning models, ranging from simple linear models to intricate deep learning models. Furthermore, SHAP offers diverse visualization tools like summary plot, dependence plot, and force plot to facilitate a comprehensive understanding of prediction explanations [33].

The main contents of the paper are as follows.

(1) The primary focus of this research paper pertains to the intentional delineation of its contents, centering on the utilization of modeling techniques aimed at forecasting the temperature of calcine within the operational framework of a rotary kiln. Specifically, the data employed in this study emanate from the RK-EF process that facilitates the production of ferronickel. Through a meticulous analysis, the model that demonstrates the highest level of accuracy in predicting the calcine temperature is identified, followed by a comprehensive elucidation of the underlying reasons for its efficacy.
(2) In the pursuit of enhancing the precision of calcine temperature prognostication, a meticulous examination of the various factors influencing this predictive process is conducted for each model under consideration. This analytical endeavor is facilitated by the application of SHAP techniques within the realm of XAI, leading to the derivation of pivotal insights into the dynamics governing the forecasted calcine temperature.
(3) To validate the reliability and robustness of the model exhibiting the most superior predictive capability in terms of calcine temperature, a meticulous verification process ensues. This verification methodology entails a comparative analysis of the deviations observed in the predicted changes in calcine temperature with the actual operational fluctuations recorded in the existing system. Furthermore, the objective is to achieve improvements over the existing operational standards by applying the optimal values of the key factors identified through SHAP analysis to the operations.

The main contributions in this paper are as follows.

(1) A model that best predicts the calcine temperature using operational data from a rotary kiln producing ferronickel with actual nickel laterite was developed, and the rationale for its superior performance was provided. This model could be utilized in future research related to predictive models using operational data in the field of pyrometallurgy.
(2) Using XAI-based SHAP analysis on the best model, the key factors contributing most significantly to the prediction of calcine temperature were identified. These insights could be applied in future operations to maintain calcine temperature and reduce variations.

The rest of this article is organized as follows. Section 2 describes the rotary kiln process and XAI, and Section 3 contains information about materials and methods. Section 4 presents the details of the experimental results. And Section 5 concludes the study.

2. Rotary Kiln Process and XAI

2.1. Rotary Kiln Process

The RK-EF process, used to produce ferronickel from laterite ore, involves a process in which a rotary kiln is utilized to elevate the temperature of calcine, eliminating nickel ore adhesion and crystalized moisture. This results in a reduction of the energy needed in the subsequent electric furnace process. The primary components of a rotary kiln include a burner system, kiln body, and exhaust-gas treatment system. The burner system is responsible for providing heat for the combustion of a reducing agent mixed with the nickel ore inside the kiln body. Various heat sources such as LNG, oil, and pulverized coal are utilized for this purpose. The kiln body is lined with refractory material to ensure longevity at high temperatures. In inclined rotary kilns, nickel ore is transformed into calcine after rotation and is discharged after undergoing drying and preliminary reduction processes within. Some rotary kilns feature a scoop feeder, a device used to separately introduce a reducing agent into the kiln body. This agent extends the high-temperature zone of the kiln, enhancing the degree and temperature of the preliminary reduction process. Additionally, an environmental offgas treatment facility is necessary to address air pollutants like NOx, SOx, and dust emitted during the combustion and processing phases in the rotary kiln. Efforts are required to minimize NOx emissions by reducing the amount produced by the burner within the kiln. If NOx levels surpass environmental standards, removal through facilities like SCR becomes essential. Roughly 30% of the sulfur content in the fuel and raw materials employed in the rotary kiln is released as SOx and can be eliminated through

environmental treatment systems like SDR and Scrubber. Dust removal is commonly carried out using cyclone and bag filters.

2.2. XAI

XAI, also known as eXplainable Artificial Intelligence, proves to be a valuable approach in elucidating the rationale behind decision-making processes that stem from the outcomes generated by artificial intelligence models [34]. XAI is a technique that adds explainability to artificial intelligence models, allowing us to understand the rationale behind the decisions made by the model when reaching a specific conclusion. The term 'explanatory power' refers to how well people can comprehend the basis of the decisions made by the AI model. As the number of data, like the number of features, increase, the issue of complexity becomes more pronounced. XAI can help mitigate these complexity issues, enabling us to trust the system's output and confidently use AI for future decision-making. For this reason, XAI is also referred to as 'Interpretable AI' or 'Transparent AI'.

We aim to utilize the SHAP method, one of the XAI techniques, to extract key variables that influence the preliminary reduction process in the rotary kiln and aid in process management and calcine temperature prediction.

2.3. SHAP

SHAP (SHapley Additive Explanations) is a technique based on game theory that expands its applicability by allowing additive usage grounded in the independence of variables. Shapley values quantify how much each variable contributes to the overall prediction. According to Shapley values, the contribution of each variable can be represented by the extent of change in the overall prediction when the contribution of the variable is excluded [35].

Shapley values can be negative, in which case it can be interpreted that a particular feature has a negative impact on the prediction. If the value is positive, it indicates that the feature is positively influencing the prediction. SHAP has characteristics that can overcome the drawbacks of other XAI techniques, such as Feature Importance and Partial Dependence Plots (PDPs). Feature Importance is a technique that identifies the variable that has the greatest impact on the prediction, by permuting it. Permutation involves randomly changing the value of each feature in turn and measuring the effect of that change on the prediction. While this method is powerful, the importance can vary with each execution of the algorithm due to the limitations of the permutation process and error-based estimation. Additionally, Feature Importance overlooks feature dependencies, so it should be avoided in models where there is a correlation between features.

Partial Dependence Plots (PDPs) work by adjusting the value of the feature of interest, inputting it into the model, and then averaging the prediction. However, PDPs have the limitation of only being able to display relationships up to three dimensions, meaning they cannot represent higher dimensions, which can lead to distorted results.

SHAP, on the other hand, calculates the impact on the model while considering feature dependencies, and has the advantage of being able to visualize even when there are many features. Given that the independent variables used to accurately predict calcine temperature have high inter-variable correlation and high dimensionality, SHAP was deemed more suitable than Feature Importance or PDP, and the analysis was conducted based on this methodology.

The SHAP methodology serves as an instrumental framework for the examination of operational datasets by augmenting the transparency of predictive models and facilitating the selection of pertinent features. Consequently, the implementation of SHAP to bolster the interpretive clarity and transparency of predictive maintenance models utilized within data centers has evidenced that quantifying the contribution of each variable permits data center managers to comprehend the model's outputs and promote anticipatory decision-making, thus enhancing both model transparency and operational efficacy [36]. SHAP has elucidated the influence of diverse variables on the incidence of expressway collisions,

demonstrating its utility for the analysis of operational data through the lens of highway-traffic safety management [37]. Furthermore, the analytical capabilities of the model were refined by evaluating the interpretability of the predictive model concerning arch dam stress, employing LightGBM in conjunction with SHAP to identify salient features impacting arch dam stress [38]. In this manner, SHAP is adeptly employed across various domains to fortify explanatory power and enhance model performance by shedding light on the determinants that affect predictive models.

3. Materials and Methods

The research methodology outlined in this paper consists of five main stages: the first stage is data collection, the second stage is data preprocessing, the third stage is model training, the fourth stage is model performance evaluation, and the fifth stage is key variable extraction and analysis of variable importance. Data collection utilized datasets from SNNC Co., Ltd. (Gwangyang, Republic of Korea). Data preprocessing considered techniques such as missing data imputation, outlier detection, and feature engineering. In the third stage, model training and forecasting were performed using Boosting-based algorithms and the GRU (Gated Recurrent Unit) method for time-series modeling. The fourth stage involved evaluating the model performance using metrics such as Mean Absolute Error (MAE), Mean Absolute Percentage Error (MAPE), and Mean Squared Error (MSE) to compare the models and select the optimal one. Finally, in the fifth stage, SHAP was applied to extract the key variables influencing the preliminary reduction process and to assess their importance, with the aim of adjusting variables to increase the calcine temperature.

3.1. Data Collection

The data used in this study were collected from the rotary kiln at SNNC Co., Ltd. The data collection period spans six months, from 1 April 2023, to 30 September 2023, with minute-by-minute data. The independent variables used can be found in Table 1; however, due to corporate security concerns, only about 6 variables will be disclosed, with the dependent variable being the calcine temperature. In this paper, we aim to propose a methodology to improve the calcine temperature in the rotary kiln preliminary reduction process by training models on the rotary kiln data, identifying key variables influencing the process using the SHAP technique, and evaluating the impact of these variables, to implement improvements in operations.

Table 1. Main independent variables of rotary kiln-process data.

Independent Variable	Unit	Independent Variable	Unit
Moisture content of the ore	%	Dried-ore feed rate	ton/h
Inner temperature of rotary kiln	°C	Reductant-coal unit consumption	kg/dmt
Coal-feeding ratio through a scoop feeder	%	O_2 content in the offgas	%

3.2. Data Processing

The most critical step in data analysis is data preprocessing. In particular, handling missing values due to equipment malfunctions or human errors, and addressing outliers caused by scheduled maintenance, clinker discharge, and other factors are essential pre-processing tasks. Preprocessing can also involve removing or replacing highly correlated variables, eliminating variables with similar meanings, and generating derived variables.

3.3. Model Training

To predict calcine temperature, four algorithms were employed: XGBoost, LightGBM, CatBoost, and GRU.

3.3.1. XGBoost

XGBoost is designed to enhance the speed and accuracy of Gradient Boosting Machines (GBMs). It features rapid training through parallel processing, a flexible learning system, overfitting prevention, and scalability for various scenarios. XGBoost adds a regularization term to the objective function to prevent overfitting and optimizes it quickly using second-order Taylor approximation. The algorithm uses an approximate method for finding the best split based on the percentile of feature distributions, which is more efficient than the exact greedy algorithm (EGA). It also addresses data sparsity with a sparsity-aware split and reduces the cost of sorting data for tree learning through a block structure in the in-memory unit, enabling parallel processing and supporting column subsampling. XGBoost has three main features.

3.3.2. LightGBM

LightGBM was developed to address the efficiency issues of XGBoost. It maintains the accuracy of previous algorithms while offering improved efficiency, being notably lightweight. LightGBM, based on Gradient-Boosting Decision Tree (GBDT), is a powerful algorithm in terms of computational complexity. Unlike traditional GBDT, which requires accessing all features and data, LightGBM employs Gradient-based One-side Sampling (GOSS) and Exclusive Feature Bundling (EFB) to reduce computational complexity. GOSS balances the reduction of data instances with maintaining accuracy, and EFB groups' mutually exclusive features, to increase training speed without sacrificing accuracy.

3.3.3. CatBoost

CatBoost is an algorithm which is effective for handling categorical variables. To prevent data leakage, it uses Ordered Target Encoding and Ordered Boosting, which helps prevent overfitting due to the Random Permutation that shuffles the order of the data in the training set. In addition to these features, CatBoost efficiently encodes categorical features using multiple characteristics and integrates them into the boosting process, reducing predictive shift and improving model performance.

3.3.4. GRU

GRU (Gated Recurrent Unit) is a type of Recurrent Neural Network (RNN) designed to solve the vanishing gradient problem and is a simplified version of Long Short-Term Memory (LSTM), with fewer parameters, often resulting in faster training times while maintaining performance. The GRU model is a type of RNN designed to address the long-term dependency problem associated with gradient vanishing. GRU enhances RNN by adding a cell state to the hidden state, allowing it to consider more past data and make more accurate future predictions.

3.4. Model Evaluation

To evaluate whether a model can effectively extract variables that explain key factors influencing calcine temperature prediction, the model's performance is compared using three primary evaluation metrics: MAE, MSE, and MAPE. MAE, which is the mean absolute error, is calculated by taking the absolute difference between the actual and predicted values, summing them up, and then averaging them. This metric is particularly useful when dealing with a high number of outliers. MSE, or mean squared error, is obtained by squaring the difference between the actual and predicted values and then averaging the results. MAPE, the mean absolute percentage error, expresses MAE as a percentage, addressing the issue of scale dependency in error measurement. Finally, MLSE is an evaluation index that calculates the mean by squaring the logarithmic difference between predicted and real values.

$$MAE = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - \hat{y}_i\right)^2 \quad (1)$$

$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left|y_i - \hat{y}_i\right| \tag{2}$$

$$MAPE = \frac{100\%}{n}\sum_{i=1}^{n}\frac{\left|y_i - \hat{y}_i\right|}{|y_i|} \tag{3}$$

$$MLSE = \frac{1}{n}\sum_{i=1}^{n}\left(log\left(\hat{y}_i\right) - log(y_i)\right)^2 \tag{4}$$

3.5. Extraction of Key Variables

The Shapley value has the advantage of revealing the importance of each variable based on combinations of multiple independent variables, and it also allows us to understand the positive or negative impact of each variable. For example, if the Shapley Value of a certain independent variable is negative, it indicates that the variable lowers the calcine temperature, while a positive value suggests that it increases the calcine temperature. In this study, we aim to identify the key variables influencing the calcine temperature using the SHAP technique, focusing on the variables collected from the preliminary reduction process in the rotary kiln.

4. Research Experiment and Results

4.1. Datasets

This study utilized minute-by-minute operational data spanning six months, from 1 April 2023, to 30 September 2023, from SNNC Co., Ltd. A total of 115,619 data points were used. After data preprocessing, the training data consisted of approximately 94,019 data points from 1 April to 31 August, while the test data consisted of approximately 21,600 data points from September 1 to September 30. Due to corporate security concerns, the exact number and nature of the 30 explanatory variables cannot be disclosed. However, key variables such as temperatures at various positions of the rotary kiln, reductant-coal feed rate, and NOx concentration in the offgas were employed, based on the expertise of operational specialists, to predict the dependent variable, calcine temperature. A summary of the rotary kiln dataset is presented in Table 2, and an example of the rotary kiln data is provided in Table 3.

Table 2. A summary of rotary kiln dataset.

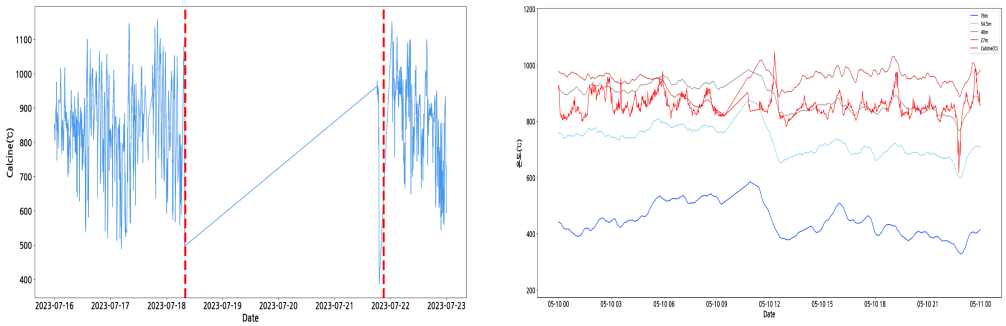
Description		Variable Name
Explanatory variables	27m (°C), Reductant feed rate, NOx etc.	X01, . . ., X30
Response variables	Calcine temperature (°C)	Calcine temperature (°C)

Table 3. Examples of variables.

Date	X1	X2	. . .	Calcine Temperature (°C)
1 April 2023 00:01:00	36.22	−1.45	. . .	925
1 April 2023 00:02:00	36.23	−1.39	. . .	930
. . .	. . .	. . .	. . .	943
30 September 2023 23:57:00	46.13	−0.96	. . .	722
30 September 2023 23:58:00	47.86	−0.69	. . .	714
30 September 2023 23:59:00	47.86	−1.15	. . .	691

4.2. Outlier Detection and Missing Values Handling

Due to the nature of the smelting industry, which utilizes naturally sourced raw ore, there is significant variability in the operational data which are shown in Figure 1.



(**a**) (**b**)

Figure 1. Raw operation data with variabilities and noises. (**a**) Example of regular maintenance period and calcine temperature (°C); (**b**) example of calcine temperature (°C) with different patterns and temperatures (°C).

The primary objective of this study is to accurately predict the minute-by-minute calcine temperature. Given the inherent variability and noise in the raw operational data, immediate analysis is not feasible. Therefore, we performed three types of data preprocessing before proceeding with the analysis.

First, we addressed missing values. Each variable had missing values, and we employed different imputation methods based on the characteristics of each variable. Specifically, missing values caused by equipment anomalies or unclear reasons were replaced with the preceding values. For the rotary kiln internal temperatures, which exhibited high inter-variable correlations, we used regression imputation.

Second, we handled outliers. There were two types of outliers: those with identifiable causes and those without. We employed rule-based outlier detection, replacing outliers with the 10 min average or median values preceding the outlier. Notably, for the dependent-variable calcine temperature, outliers often occurred due to clumping of calcine inside the kiln, clinker discharge, scheduled maintenance, or other operational patterns causing sudden temperature drops. Consequently, we removed instances where values continuously fell below a specific threshold.

Third, we generated derived variables and identified relationships between variables to reduce dimensionality. New variables were generated by combining existing variables with new derived variables that were not originally present in the data. Additionally, variables with comparable meanings were eliminated if they exhibited lower correlation coefficient values in relation to the dependent variables.

Before the above three steps of data processing, the average MAE value of each model was near 60–70 °C, but after the pre-processing, it was confirmed that the average MAE value of the model was very low, and that it was 38–45 °C. In particular, the outlier treatment of variables related to temperature, coal, and ore contributed greatly and had the advantage of being able to clarify the relationship between variables in terms of interpretation. For example, processing the percentage outliers of ore components resulted in the same correlation between components from 0.8 to 0.2, which was equivalent to the theoretical results. One of the temperature variables included, periodically, outliers of 0 and 1, and replacing the above values with the previous values resulted in significant results for the performance of the model.

4.3. Model Training for XAI

The purpose of this study is to accurately predict the calcine temperature and extract and identify key variables influencing calcine temperature predictions. The dependent variable is calcine temperature, and the independent variables consist of 30 variables collected from the rotary kiln. In this study, the training data cover the period from 1 April to 31 August 2023, while the test data span the month of September 2023. The goal is to predict approximately 21,600 data points. Modeling was performed using boosting

models such as XGBoost, LightGBM, and CatBoost, and predictions were made using the deep learning time-series model GRU. To prevent overfitting, 5-fold cross-validation was employed, and Bayesian optimization was used to optimize the hyperparameters.

There are three main reasons for choosing boosting-based models.

First, preventing overfitting and ensuring model stability. Boosting models, built on tree-based structures and regularization techniques, are highly effective at preventing overfitting. The Shapley values derived from such models can reflect these characteristics as well. In contrast, deep learning models tend to be more sensitive to overfitting, especially in cases involving small Shapley values, which may lead to instability. However, boosting models provide relatively more-stable feature importance.

Second, enhancing model interpretability. Deep learning models, often characterized as black-box models, offer limited interpretability. Boosting models, however, are more interpretable, and when combined with Shapley values, they can clearly explain the effects and interactions between features. This makes boosting models advantageous for interpretation.

Third, balancing performance and explainability. While deep learning models can deliver excellent performance, they often lack explainability. On the other hand, regression models are easy to interpret but may underperform with complex data. Boosting models strike a balance between performance and interpretability. Moreover, the Shapley values extracted from these high-performing models contribute to enhancing their interpretability.

4.4. Performance Result of Models

The performance results of the XGBoost, LightGBM, CatBoost, and GRU models are shown in Table 4. CatBoost outperformed all other models across all evaluation metrics (MAE, MSE, MAPE, and MLSE). Based on these comparison results, CatBoost was selected as the model to be used for the SHAP technique to extract and identify key variables.

Table 4. Model evaluation-metric results.

Model	MAE	MSE	MAPE	MLSE
XGBoost	41.73	2539.72	0.045	0.0047
LightGBM	39.24	2575.97	0.040	0.0062
CatBoost	38.22	2500.36	0.036	0.0038
GRU	48.13	3200.14	0.079	0.0084

4.5. Extraction Results of Key Variables

The SHAP method, a technique in XAI was employed to analyze the variables used in the prediction model. The primary variable identified was X10, and the top 10 variables collectively explained a significant percentage of the model's predictive power. Specifically, the SHAP analysis revealed that when certain variables increase or decrease, the calcine temperature correspondingly rises or falls. Variables X10, X9, and X22 were among the highest contributors to the model's predictions, indicating their substantial impact on the calcine temperature. The SHAP analysis not only identified the most influential variables, but also elucidated their directional impact on the calcine temperature, enhancing the interpretability and transparency of the prediction model.

The primary factors that influenced the comprehensive predictive model were prioritized as follows: X10, X9, X15 and X8, as shown in Figure 2. The thermocouples, which measure the inner temperature of the rotary kiln positioned nearest to the calcine outlet, exhibit the strongest correlation with the calcine temperature. This relationship can be attributed to the impact of calcine temperature, supplied by the burner, on the NO_X, O_2 components of offgas. Additionally, the rotation speed of the rotary kiln RPM influences the duration that the ore remains in the kiln after being fed through the inlet.

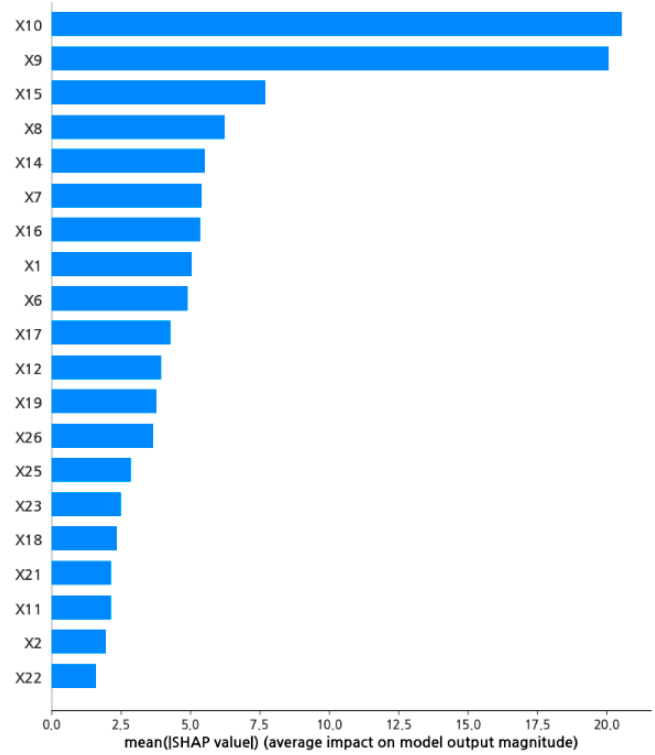


Figure 2. Mean of SHAP values.

Moreover, we compared the variability in calcine temperature changes under this preemptive control with the variability observed in conventional operations. An increase in X10, X9, and X8 had a positive effect on the increase in calcine. In addition, as shown in Figure 3, an effect of decreasing the calcine temperature was observed as the variables such as X14, X7, and X12 increased.

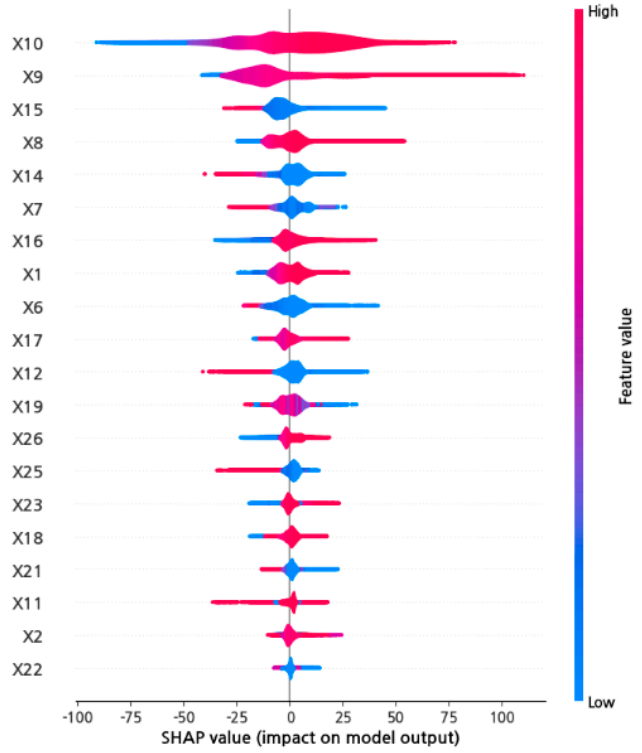


Figure 3. SHAP values with different variables.

Upon closer examination, the operating factors identified by SHAP reveal connections with calcine temperature. Nevertheless, SHAP's variable interdependence analysis elucidates the impacts and directions of variables influencing calcine temperature, despite potential interactions among them. The objective is to explore the effects of derived variables on calcine temperature. To elevate calcine temperature, effective combustion of the burner's heat source is essential. The burner's heat must facilitate the combustion of the reducing agent with the ore in the rotary kiln to achieve reduction and temperature elevation. Due to inadequate heat transfer and exchange with the ore, excess heat is expelled as exhaust gas; thus, optimizing the ore's residence time in the rotary kiln by adjusting RPM while maintaining rotary kiln body temperature is vital. Additionally, excessive heat from the burner can raise the flame-tip temperature and NO_X emissions to the offgas [39]. Nevertheless, when rotary kiln body temperature is adequately managed, the overall NO_X output can be minimized by curtailing emissions from the reducing agent's combustion. By fine-tuning key operational parameters from X10 to X17 identified by SHAP, the rotary kiln's reaction mechanism was optimized, enabling precise targeting of calcine temperature.

In conclusion, the SHAP method identified the key factors impacting calcine temperature, and preemptive control of these factors demonstrated a reduction in temperature variability compared to standard operational practices, confirming the model's efficacy.

5. Conclusions

This paper studies aimed to predict calcine temperature and identify influencing factors using XAI's SAHP to address rising power costs linked to renewable energy and fossil fuels. Temperature predictions were executed utilizing XGBoost, LightGBM, CatBoost, and GRU algorithms. The prediction accuracy was highest with CatBoost, achieving a MAPE of 0.036, followed by XGBoost at 0.045, LightGBM at 0.040, and GRU at 0.079. Using XAI's SAHP with CatBoost, we derived influential factors impacting calcine temperature based on its superior predictive performance. Typically, rotary kiln operations sustain optimal conditions by adjusting parameters informed by expert experience; however, variability in nickel laterite composition necessitates precise identification of factors to maintain calcine temperature stability. By implementing SHAP-derived variables X10, X9, X15, X8, X14, X7, and X16 from April 2024, the average calcine temperature rose from 840 °C in 2023 to 910 °C, enabling a 7.8% reduction in electric furnace power units and lowering manufacturing costs while electricity cost increased 10.2% in Republic of Korea.

While the CATBoost algorithm and SAHP have achieved successful predictive outcomes, further enhancements in accuracy and adherence to established model standards are vital for real-world application. Efforts ought to be aimed at refining the predictive capabilities of models that govern the operational characteristics of autonomous rotary kilns. Key operational variables, identified via XAI's SHAP methodology, significantly influence calcine temperature management. A pivotal operational variable also impacts calcine temperature, due to concurrent chain reactions within the rotary kiln. Consequently, operators face challenges in intuitively recognizing the key operating variables that influence calcine temperature. Nonetheless, enhancements in the CATBoost algorithm to augment predictive performance, coupled with the determination of optimal variable values through Bayesian optimization, may support the delivery of reference values for rotary kiln operators via HMI. By regulating calcine temperature and minimizing electric furnace power consumption according to the predictive model's guide values, autonomous operation of the rotary kiln could be achieved through manual input into the PLC.

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Conflicts of Interest: Author Mr. Seongil Mun is employed by the company SNNC. The remaining authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as potential conflicts of interest.

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