# A soft measurement model construction method based on machine learning and CFD

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The computational fluid dynamics (CFD) of traditional metallurgical numerical simulation is generally a large amount of time cost consumption, which cannot be real-time response and poor traceability. In contrast, the data-driven soft measurement-based model can effectively solve the problem of time response during CFD simulation and achieve real-time prediction and optimization of metallurgical production processes. Therefore, this study proposes an AI-based prediction and optimization method to accelerate CFD simulation and assist in constructing a soft measurement model for metallurgical processes. This method combines machine learning and CFD simulation techniques to achieve real-time prediction and optimization of metallurgical processes by learning and analyzing offline collected data. At present, the method has been successfully used in metallurgical processes such as rotary kiln and shaft furnace, and through the AI analysis of the collected temperature field and flow rate field data, it effectively optimizes the quality of the products during the operation of the rotary kiln and shaft furnace. And the method is expandable, not only limited to specific special and field information, so it has a broad development and application prospects. By introducing soft measurement technology and artificial intelligence methods, the efficiency and quality of metallurgical production can be further improved, and the metallurgical industry can be promoted to develop in the direction of digitalization and intelligence.

**KEYWORDS:** COMPUTATIONAL FLUID DYNAMICS, MACHINE LEARNING

## INTRODUCTION: HEADING

The rotary kiln, as an important industrial equipment [1], are widely used in industries such as metallurgy and mining [2]. However, it represents a nonlinear, multivariable, strongly coupled system, typical of a "black-box" reactor [3]. The temperature field within the kiln is easily influenced by various factors such as material reaction thermodynamics, heat transfer, mass transfer, and material movement states[4], leading to the occurrence of ring formation, resulting in increased energy consumption and decreased product quality [5]. Therefore, there is an urgent need to explore advanced temperature sensing and optimization technologies to extend the operational lifespan of rotary kilns and enhance product quality [6,7].

Regarding temperature sensing technology, scholars have conducted a large amount of research. Currently, temperature sensing technology can be primarily classified into two categories: 1) Instrumentation-based hard measurement methods; 2) Modeling [8], simulation [9], and algorithm-based [10] soft measurement

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methods. In the realm of traditional hard measurement methods, in traditional hard measurement, manual timing measurement of the rotary kiln shell temperature is one of the main methods for detecting the kiln temperature.

This study proposes an integrated predictive and optimization system for monitoring the temperature of rotary kilns. This method combines the precision of CFD [11] with the speed of machine learning and optimization algorithms, providing guidance for frontline workers in optimizing the temperature field of rotary kilns in industrial settings. By expanding the dataset, the accuracy of predictions can be improved. this paper utilized 625 sets of case generated by the design of experiments (DoE) for database storage in the data preparation stage, ensuring the accuracy of subsequent prediction and optimization models. Initially, structural parameters for temperature field optimization were determined. Subsequently, the data in the database were standardized, and four different ML models were trained. The best-performing random forest (RF) model was ultimately selected as the model for predicting the overall temperature field of the rotary kiln. In the optimization part, the RF was reused to construct two objective function models (calcination zone width and maximum temperature in the region). These models were then used as inputs for the R-NSGA-II to obtain parameter optimization solutions. Then verification was conducted using CFD models, followed by Pareto solution set evaluation based on the TOPSIS to select the optimal solution. This study provides DMs in industrial settings with a solid theoretical foundation and important reference. It is important to note that the optimization method is scalable and not limited to temperature field optimization of rotary kiln equipment. By collecting data from different CFD models, it is also possible to estimate different parameters of various equipment such as flow fields in vertical furnaces. Exploring these applications is a direction for future research.

## TECHNOLOGY METHOD

To reduce labor costs and save time in optimization, this study has established an integrated system combining CFD, ML, NSGA-II, and TOPSIS. This predictive optimization system consists of four modules: (1) the CFD model, (2) the machine learning prediction module, (3) the R-NSGA-II optimization module, and (4) the TOPSIS module. Each of these modules will be detailed subsequently.

In this study, under pre-defined conditions, Design of Experiments (DoE) was used to design the experimental variables, and Computational Fluid Dynamics (CFD) simulations were conducted for 625 cases to establish a database of the temperature field distribution throughout the rotary kiln. The rotary kiln model developed in this article comprehensively considers the complex combustion processes within the kiln, such as turbulent particle flow and mass and momentum equations. Therefore, the CFD model has high reliability and can be used for subsequent research work. Below is a detailed description of the dataset and modeling process.

To simulate the temperature field distribution throughout an industrial-scale rotary kiln, a model was developed in ANSYS Fluent. First, a two-dimensional planar model file was created for a rotary kiln that is 40 meters long and has a cylinder diameter of 6 meters. This model was determined on a 1:1 scale according to specifications from a steel company, and actual values will be compared with simulation results to ensure the authenticity of the simulation outcomes. Following this, the prepared model file was imported into the ANSYS meshing software for grid generation. To accelerate the convergence of the model, hexahedral grids were used instead of tetrahedral grids. Due to intense turbulence and flow fluctuations near the burner, the surrounding region was subjected to grid refinement.

## ML MODEL PREDICTION RESULTS

To validate the reliability of the CFD simulations, this study compared them with measurements obtained from thermocouples in the actual plant. Due to equipment limitations during real-world temperature measurements, only the temperatures at the kiln head and kiln tail could be measured. Therefore, these temperatures served as the baseline values for error comparison. Some of the measured values are shown in Table 1. From Table 5, it can be seen that the CFD simulation results have good consistency with the experimental data, with the maximum error between the experimental values and the CFD simulation values not exceeding 10°C. This indicates that using these CFD datasets for ML prediction and optimization decision-making in subsequent studies is reasonable.

**Tab.1** - Rotary kiln true value and simulation value error table.

| Rotary kiln temperature measurement area, °C | Rotary kiln head | Rotary kiln tail |
|---|---|---|
| Experiment | 1100.00-1110.00 | 1000.00-1010.00 |
| CFD | 1109.28 | 1012.48 |
| Error | 0.72-9.28 | 2.48-12.48 |

The initial parameters for four ML methods were set. The selection and range of hyperparameters were determined based on a combination of grid search and experience. It can be seen that after optimization, the $R^2$ values of the models have improved, with all four algorithms achieving an $R^2$ of 0.90 or higher, indicating a high level of fit accuracy. Among them, the RF model performed the best, reaching an optimized $R^2$ of 0.999. Therefore, the RF model was selected as the predictive model for the temperature field of the rotary kiln. According to the method outlined in Section 2, the analysis and validation of the ML models were conducted, resulting in the actual versus predicted values of the coupled CFD-ML surrogate model. All four ML models were relatively accurate in predicting the temperature field distribution of the rotary kiln, with the error in each grid point inside the kiln not exceeding 5°C, indicating high predictive accuracy. However, the CNN model had slightly higher error values. The RF model had the best predictive performance among the four models, ensuring good prediction accuracy even in high-temperature regions.

Table 2 provides a quantitative analysis of the four models, showing the MSE, MAPE, and $R^2$ values of the prediction results. The accuracy of the models depends to some extent on the distribution of the dataset. In the dataset distribution of this study, the RF model has the lowest values for MSE, MAPE, and the highest $R^2$. This indicates that for predicting the temperature in the rotary kiln, using the Random Forest model for feature extraction in this dataset is more effective and can achieve precise measurements with more stable numerical performance. Considering the stability and precision of the predictive capabilities for subsequent use, the RF model was chosen as the predictive model for the temperature field of the rotary kiln.

**Tab.1** - Model evaluation of four ML methods

| ML model | BP network | Random Forest | XGBOOST | CNN |
|---|---|---|---|---|
| MSE | 60.73331 | 0.02295 | 0.80769 | 182.96543 |
| MAPE | 1.91123 | 0.00327 | 0.04083 | 3.51779 |
| R-Square | 0.99946 | 0.99999 | 0.99994 | 0.99427 |

## CONCLUSION

This paper proposes a predictive model for the temperature field in rotary kilns based on machine learning coupled with Computational Fluid Dynamics (CFD) and a multi-objective optimization method based on an improved NSGA-II algorithm. This approach optimizes the width of the calcining zone and the highest temperature within the region to improve the overall temperature distribution in the rotary kiln. The study first screens and preprocesses data and key variables, then uses a series of machine learning methods to predict the performance of the temperature field. Finally, the optimization algorithm is applied to optimize the temperature field across the entire domain of the rotary kiln, and the Technique for Order of

Preference by Similarity to Ideal Solution (TOPSIS) is used to evaluate and select the best solution from the Pareto front. The accuracy of the optimization is validated using a CFD model. The main conclusions are as follows:

(1) Factors influencing the distribution of the temperature field inside the rotary kiln were identified. An analysis was conducted on the effects of four variables—volatile matter content, secondary air temperature, secondary air velocity, and coal injection rate—on two objective functions: the width of the calcining zone and the highest temperature in the region. A full factorial analysis of experiments (DoE) was then used to generate combinations of these five variables for CFD simulations, which served as a real baseline for subsequent studies.

(2) A prediction of the temperature field across the entire domain of the rotary kiln was performed. Four ML models were used to predict the temperature field, and the results showed that the Random Forest (RF) model was considered the most suitable machine learning model for this dataset, with evaluation metrics of MSE = 0.023, MAPE = 0.003, and $R^2$ = 0.999, indicating a reasonably good prediction performance.

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