

# Syngas Calorific Value Prediction for Underground Coal Gasification Based on Informer

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**Abstract:** Coal property and operational parameter variations cause, the underground coal gasification (UCG) systems to exhibits diverse gasification processes. As gasification reactions persist, the secondary combustion proportion of combustible gases, increases, leading to unstable gasifier reaction states. Consequently, the composition and calorific value of syngas decline after a stable production period, necessitating the intervention of new control methods to prevent further deterioration. This study proposes eight characteristic variables that influence the calorific value of syngas based on the mechanism analysis of the UCG process. Through similar simulation experiments, datasets were collected for UCG under various characteristic variables. Using the Pearson analysis results from high-quality datasets, different input combinations were established, and a syngas calorific value prediction model was proposed. The model's performance was evaluated from different perspectives using three evaluation metrics: RMSE, MAE, and  $R^2$ . The prediction performance was studied under three types of gasification channels, three sampling frequencies, and four prediction lengths. The results indicate that the Informer model performs well with optimal input. In long-sequence predictions, the  $R^2$  value under optimal input exceeds 80%.

**Keywords:** Underground coal gasification (UCG); Pearson; Informer; Syngas calorific value Prediction.

## 1. Introduction

Underground coal gasification (UCG) is an advanced technology for cleanly utilizing coal. This process involves the direct partial underground combustion of coal to produce clean, combustible syngas that is primarily composed of  $H_2$ ,  $CO$ , and  $CH_4$ , thus effectively bypassing the traditional coal combustion process [1,2]. This technology achieves controlled chemical reactions by injecting gasifying agents, thereby enhancing energy efficiency while significantly reducing sulfur and nitrogen oxide emissions [3]. Compared to conventional coal mining methods, UCG minimizes surface disruption and environmental pollution, making it suitable for deep, steep, or gently inclined coal seams and reducing mining costs [4]. Furthermore, the development of UCG technology aligns with national strategies for building a low-carbon, clean, safe, and efficient modern energy system, offering broad application prospects and significant environmental benefits [5-7].

However, UCG technology still faces several challenges in large-scale commercial applications, such as unstable gas yields and calorific values, low gasification efficiency, and a small proportion of combustible gases that are easily volatile [8]. These factors limit the application scope of UCG products and the effectiveness of industrial prediction methods. To enhance the operational stability of a UCG system, predicting the calorific value of syngas becomes particularly crucial. This not only aids in understanding the operational status of the system but also guides subsequent control measures for optimizing the gasification process [9]. By controlling the flow, composition of gasifying agents, and pressure within the reactor, the stability of the UCG process can be improved to some extent [10]. Therefore, predicting the calorific value of syngas is highly important for improving the reliability of UCG technology and promoting its commercial application.

In recent years, scholars from various countries have conducted extensive theoretical and experimental research on

predicting the UCG gasification process, the developed approaches can be categorized into theoretical model predictions and experimental data prediction methods. Theoretical Model Prediction Methods: Jowkar Amin et al. [11] proposed a model based on a series of equations and cavity pressure and temperature information to predict the dynamic cavity shape and volume changes induced during the underground gasification process. Using COMSOL software for numerical simulation purposes, the model accurately predicts the cavity shape and volume during the initial gasification stages. Otto Christopher et al. [12] employed a thermochemical equilibrium modeling method to predict the composition of syngas in UCG. Dufaux et al. [13] utilized chemical equilibrium on the coal surface to predict gas compositions. However, this model overestimates the concentration of carbon monoxide and underestimates the carbon dioxide content in the product gas. Laciak et al. [14] calculated the concentrations of gasification products obtained at different gasification temperatures using the known temperature and pressure of UCG while, employing Gibbs energy minimization- and Lagrange multiplier-based finite optimization methods. However, this method only accurately predicts the concentration of a single output gas under one temperature condition, with significant deviations induced when predicting other gas concentrations. Eftekhari et al. [15] extended existing steady-state models to transient models capable of describing the alternate injection of air and steam into deep thin coal seams. Experimental results showed that this model could predict gas compositions more accurately than the aforementioned models. Subsequently, the authors validated the model on field test data, confirming the accuracy of its gas composition predictions. Overall, the theoretical model prediction methods for UCG have lower accuracy than that of other techniques, focus on the final syngas composition and concentration, and are unable to provide real-time predictions. Experimental Data Prediction Methods: Durdán Milan et al. [16] explored the possibility of

predicting temperature data in UCG experiments, by proposing regression models with different structures for visualizing the growth of gasification cavities. Najaf Mehdi et al. [17] developed a new model using multivariate regression analysis to predict the cavity growth rate (CGR) during UCG. The researchers collected data from 11 UCG field tests and constructed an empirical model using nonlinear regression analysis. This model accurately predicted the CGR and demonstrated greater predictive reliability than did the Perkins model. Kaur et al. [18] used support vector machine methods to predict calorific value and temperature data obtained under laboratory conditions in UCG experiments. Krzemien Alicja et al. [19] developed a temperature prediction model using multivariate adaptive regression splines (MARS) to predict the fire risk encountered during UCG. Xiao Yuteng et al. [20] proposed a dual-source long short-term memory (LSTM) prediction model to for predicting UCG statuses and achieved better prediction accuracy than that of the existing methods, with a maximum equivalence trend prediction accuracy of 90.99%. Compared to theoretical model predictions approaches, experimental data prediction models for UCG enable online real-time prediction capabilities and offer greater accuracy.

The transformer model [21], which is a deep learning model, has been widely applied in the natural language processing (NLP) and computer vision (CV) fields. Some scholars believe it has the potential to provide enhanced prediction capabilities. However, due to its high time complexity, high memory utilization rate, and drastic prediction rate decrease, it cannot be directly applied to time series forecasting scenarios. Numerous scholars have made significant efforts to address these issues, by proposing various methods. Child Rewon et al. [22] considered sparsely decomposing the attention matrix. Li Shiyang et al. [23] proposed the logsparse transformer by, introducing a convolutional self-attention mechanism. Beltagy Iz et al. [24] introduced an attention mechanism called Longformer that scales linearly with the input sequence length. Wang Sinong et al. [25] proposed a new self-attention mechanism that reduces the complexity of self-attention across time and space. Zhou H et al. [26] designed an efficient transformer-based LSTF model, named Informer. Extensive experiments conducted on four large-scale datasets showed that the Informer algorithm significantly outperformed the existing methods, providing a new solution to the LSTF problem.

UCG data exhibit high-dimensional, nonlinear, and nonstationary time series characteristics, which can hinder traditional time series forecasting models [27]. The Informer model, which is a time series forecasting model based on self-attention mechanisms, can effectively handle high-dimensional and complex time series data. Therefore, investigating the ability of the Informer model to predict the calorific values of UCG syngas is highly important. To the best of the author's knowledge, the previous research on UCG syngas calorific value prediction focused primarily on theoretical models for obtaining short-sequence predictions, with limited related studies and applications. Research on applying the Informer model in this field is lacking. To explore the performance of the Informer model in terms of predicting the calorific value of UCG syngas, this study used laboratory-acquired UCG syngas calorific value data as an example. Through simulated experiments, experimental UCG data were collected for different gasification channel types, and a corresponding prediction framework was established.

Subsequently, these datasets were used to train the Informer model, and its predictive performance was comprehensively evaluated by assessing the prediction accuracy achieved across different datasets. The research work conducted in this paper is outlined as follows:

(1) An in-depth analysis of the UCG mechanism was conducted to select appropriate feature variables for the input model. Simulated experiments were carried out to collect experimental UCG data for different gasification channel types. The Informer model was then used for prediction purposes, and its performance was evaluated from various perspectives using three indicators: the root mean square error (RMSE), mean absolute error (MAE), and coefficient of determination ( $R^2$ ).

(2) The data processing strategy involved checking for missing data, removing outliers, selecting key parameters, and adding necessary parameters. The input experiments were designed based on Pearson correlation coefficient results. The findings indicated that different input combinations significantly affected the accuracy of the developed model, highlighting the necessity of determining the optimal input combination.

(3) Multiple evaluation metrics were calculated across four prediction lengths to assess the predictive ability of the Informer model. Under the optimal input conditions, the Informer model consistently performed well in all scenarios. However, increasing the sampling frequency had a minimal impact on the long-sequence prediction effectiveness of the model.

(4) By integrating the prediction results of the Informer model with a statistical analysis method for determining the calorific value decline rate, the points at which the calorific value abruptly changed were identified using statistical measures such as the standard deviation and mean. This approach enabled the determination of new control measures intervention points.

## 2. Informer Model

The Informer network is one of the most advanced deep neural networks, showing significant effectiveness in many time series prediction tasks. The Informer is a time series forecasting model based on a transformer architecture that consists of an encoder and a decoder, and was designed to better capture the long-term dependencies of time series data. The encoder uses a sparse self-attention mechanism to robustly extract long-range dependencies from long-sequence inputs. Unlike traditional self-attention mechanisms, the sparse self-attention significantly reduces the temporal complexity and memory usage of the model, enhancing its efficiency in terms of handling long-sequence data and greatly reducing its computational resource consumption. An active compression model structure is employed to maintain a performance level similar to that of the original network structure while its reducing spatial complexity. This approach makes the model more efficient when addressing large-scale data. The decoder introduces a generative decoding method that obtains long-sequence prediction results through single-step outputs. This approach prevents error accumulation, which is a common shortcoming of traditional decoders during multistep prediction tasks. By incrementally generating the prediction value at each step, the generative decoder significantly improves the accuracy of long-sequence predictions.

Due to these improvements, the Informer model has demonstrated outstanding performance in many time series prediction tasks. The overall structure of the Informer model is illustrated in Figure 2, with the encoder on the left and the decoder on the right. This architecture enables the Informer to more effectively handle complex time series prediction tasks than can other approaches. By leveraging these advanced mechanisms, the Informer model efficiently processes high-dimensional, nonlinear, and nonstationary time series data that are typical of UCG processes, providing accurate and robust syngas calorific value predictions. This capability is crucial for optimizing UCG operations and maintaining high-quality syngas production.

## 2.1. Prediction Model Framework

The basic framework for of the syngas calorific value prediction model included data collection, data preprocessing, data splitting, model training, and model evaluation mechanisms.

**Data Collection:** Three different UCG simulation experiments with various gasification channels were established to collect operational data, including gasifying agent types, injection flow rates, oxygen concentrations, and syngas compositions.

**Data Preprocessing:** During the comprehensive training and testing processes, all outliers were removed from the actual operational data, and linear interpolation was used to fill in missing values. By deeply analyzing these data, the aim is was to explore the pattern variations exhibited by the syngas calorific value under different gasification channels, thereby extracting nine characteristic variables as Informer model inputs, with the syngas calorific value as the target prediction variable, as shown in Table 1.

**Table 1.** Inputs of informer.

Input	Characteristic variable
X1	Date
X2	Oxygen injection volume
X3	Synthetic gas volume
X4	Oxygen consumption
X5	Coal consumption
X6	H <sub>2</sub> content
X7	CH <sub>4</sub> content
X8	CO content
X9	CO <sub>2</sub> content
X10 (Target)	Syngas Calorific Value

**Data Splitting:** In our work, we split the dataset into training, validation, and test sets at a ratio of 7:3:1, which is a conventional data splitting strategy.

**Model Training:** The Pearson correlation between the operational parameters of each dataset was analyzed, and three input experiments were established based on the Pearson correlation result. We used the Informer model for prediction and conducted a comparative analysis of the performances achieved by the Informer model on different datasets. Additionally, we selected, compared, and analyzed the optimal input for each model. Depending on whether the input was optimal, we set different sampling frequencies and prediction lengths, to critically evaluate various aspects of the Informer model.

**Evaluation Metrics:** When measuring the performance of a prediction model, it is crucial to use appropriate statistical

indicators to evaluate the degree of fit between the predicted and actual values. These indicators include the MAE, RMSE, and R<sup>2</sup>.

MAE quantifies the average magnitude of errors between the predicted and actual values, assigning equal weight to each error.

$$MAE = \frac{1}{N} \sum_{n=1}^N |P_n - \hat{P}_n| \quad (1)$$

RMSE uses the average of the squared errors as a measure, making it more sensitive to outliers.

$$RMSE = \sqrt{\frac{1}{N} \sum_{n=1}^N (P_n - \hat{P}_n)^2} \quad (2)$$

R<sup>2</sup> reflects the quality of the model's fit to the actual data.

$$R^2 = 1 - \frac{\sum_{n=1}^N (P_n - \hat{P}_n)^2}{\sum_{n=1}^N (P_n - \bar{P}_n)^2} \quad (3)$$

where  $P_n$ ,  $\hat{P}_n$  and  $\bar{P}_n$  represent the actual value, predicted value, and mean value, respectively. Additionally, n denotes the number of samples in the dataset. The three of the evaluation metrics (MAE, RMSE) range from 0 to 1, with smaller values indicating higher prediction accuracy. The R<sup>2</sup> value ranges from 0 to 1, with higher values representing more accurate predictions by the model.

## 3. Results and Discussion

The Before starting the experiments, we conducted a Pearson correlation analysis between the features and the target variable across the three datasets. As shown in Table 2, the coal consumption level, CH<sub>4</sub> content, CO content, and CO<sub>2</sub> content strongly correlated with the syngas calorific value across all three datasets. Specifically, the p-value of the CO<sub>2</sub> content feature was highest in Test 1, while the CH<sub>4</sub> content feature yielded the highest p-values in Test 2 and Test 3, t with values of -0.969, 0.901, and 0.940, respectively. The oxygen injection volume, synthetic gas volume, and oxygen consumption level also exhibited some degrees of correlation, with the oxygen injection volume and oxygen consumption level having similar impacts on the target. In Test 3 dataset, the oxygen injection volume and consumption level were negatively correlated with the target. However, the H<sub>2</sub> content showed very low correlations in all three datasets, with p-values close to 0

**Table 2.** Pearson correlation coefficient between features and target values.

Feature	Test 1	Test 2	Test 3
Oxygen injection volume	0.471	0.481	-0.791
Synthetic gas volume	0.628	0.507	0.565
Oxygen consumption	0.485	0.426	-0.801
Coal consumption	0.767	0.521	0.719
H <sub>2</sub> content	0.283	0.216	0.284
CH <sub>4</sub> content	0.903	0.901	0.940
CO content	0.961	0.897	0.833
CO <sub>2</sub> content	-0.969	-0.792	-0.720

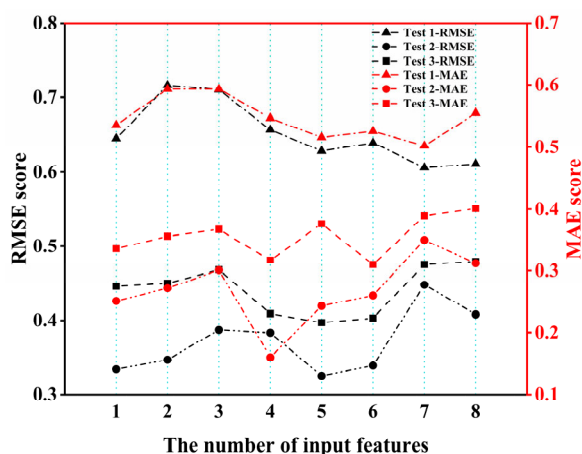
In this study, we used multiple datasets to explore the impacts of different numbers of features on the prediction performance of the Informer model. The features were selected based on their Pearson correlation p-values, and the experimental results are shown in Table 4. Additionally, Figure 5 depicts the RMSE and MAE metrics obtained for the model predictions.

According to Table 3 and Figure 1, as the number of features increased, the prediction accuracy of the Informer model also improved. When the top 5 features were selected as model inputs, the RMSE and MAE values produced for the three datasets were optimal, indicating that the chosen feature combination was beneficial for model training. However, as the number of features continued to increase, the prediction accuracies achieved on all three datasets decreased. These declines occurred because the inclusion of low-correlation features interfered with the ability of the model to capture the dependency information between the feature variables and the target value.

Based on the above analysis, this study selected five features that were highly correlated with the syngas calorific value (CH<sub>4</sub> content, CO content, CO<sub>2</sub> content, coal consumption level, and synthetic gas volume) for further experiments.

**Table 3.** Metrics of RMSE and MAE with different combinations of features

Feature number	Test 1		Test 2		Test 3	
	RMSE	MAE	RMSE	MAE	RMSE	MAE
1	0.645	0.536	0.334	0.251	0.446	0.336
2	0.716	0.593	0.347	0.272	0.450	0.356
3	0.710	0.593	0.387	0.301	0.468	0.367
4	0.657	0.547	0.383	0.160	0.409	0.317
5	0.628	0.516	0.325	0.243	0.397	0.376
6	0.639	0.526	0.339	0.260	0.403	0.310
7	0.606	0.502	0.448	0.350	0.475	0.389
8	0.611	0.555	0.408	0.312	0.479	0.401



**Figure 1.** Line plot for the MAE and RMSE metrics of the prediction results

## 4. Conclusions and Perspectives

### 4.1. Conclusions

Accurate prediction of syngas calorific value is crucial for improving the efficiency of underground coal gasification (UCG). This paper proposes a multi-sequence time series syngas calorific value prediction method based on the Informer model and comprehensively evaluates this model using nine datasets. RMSE, MAE, R<sup>2</sup>, and computation time

are chosen as evaluation metrics. The research results are explained in detail as follows:

By performing Pearson analysis to determine the correlation between features and the target, features are combined according to the p-values. When the number of feature inputs increases to five, the model's prediction accuracy reaches its optimum. Beyond this point, further increasing the number of inputs results in a decline in prediction accuracy. Therefore, identifying effective input features is crucial, as low-quality inputs can compromise a good model.

### 4.2. Perspectives

The discussion and results of this paper are of significant importance in selecting an ideal and reliable model for syngas calorific value prediction. Given the excellent performance of the Informer model in syngas calorific value prediction, our future work will focus on the following directions:

In syngas calorific value prediction, there are many factors influencing calorific value changes. It is necessary to collect more data parameters and expand the model's dataset to enable the Informer to analyze specific situations.

The ultimate goal of syngas calorific value prediction is to improve gasification efficiency. We will conduct further in-depth research on this model to study the efficiency of underground coal gasification.

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