Study on the Spontaneous Combustion Tendency of Coal Based on Grey Relational and Multiple Regression Analysis

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ABSTRACT: The correlation between the spontaneous combustion tendency of coal and its properties are of great importance for safety issues, environmental concerns, and economic problems. In this study, the relationship between multiple parameters, different from the previous single parameter, and the spontaneous combustion tendency was analyzed. The comprehensive judgment index (CJI), which indicates the tendency of coal spontaneous combustion, was obtained for samples collected from different mines. The CJI was measured by the cross-point temperature and had a negative correlation with the spontaneous combustion tendency. Physical pore structures and chemical functional groups were characterized based on cryogenic nitrogen adsorption and Fourier transform infrared spectroscopy measurements, respectively. For analyzing the effect of coal properties on the spontaneous combustion tendency, the grey relational grade was determined by the grey relational analysis between the CJI and the pore structures and functional groups of coal. The grey relational grade of the benzene substituent with CJI had a maximum of 0.8642, and the macropores had the minimum, 0.4169. The higher the gray relational grade was, the more relevant the spontaneous combustion tendency was, indicating that the benzene substituent was the most relevant. To better predict the spontaneous combustion tendency, the average pore diameter, hydroxyl, methyl, methylene, and benzene substituent with a high grey relational grade were selected. Finally, the multiple regression prediction model of CJI was established. The $R^2$ coefficient, significance level, $F$-distribution, $t$-distribution, collinearity diagnosis, and residual distribution of the model met the requirements. In addition, two coal samples were selected to verify the spontaneous combustion tendency model. The relative errors between the predicted CJI value and the experimental CJI value were 1.42 and 4.25%, respectively. These small relative errors verified the reasonableness and validity of the prediction model.

1. INTRODUCTION

Spontaneous combustion, which generally exists in coal mines, is one of the five major mine natural disasters. Additionally, spontaneous combustion of coal has caused safety accidents, economic losses, and environment issues. Hence, it is of great significance to assess the extent of the spontaneous combustion tendency for reducing spontaneous combustion of coal.

The inherent properties of coal, oxygen concentration, and moisture content are the major factors for influencing the tendency of spontaneous combustion within extremely complex physicochemical processes. Domestic and international scholars have conducted numerous studies on the tendency of coal spontaneous combustion. Nimaje and Tripathy found that the Olpinski index, which was obtained by the statistical analysis of coal parameters, could be used to evaluate the spontaneous combustion tendency of Indian coals. Pattanaik et al. concluded that the intrinsic properties of the coal (vitrinite, exinite, and inertinite) had significant correlations with the tendency of spontaneous combustion.

The tendency of coal spontaneous combustion decreased with decreasing vitrinite and exinite but increased with the decrease of inertinite content. Chandra and Prasad suggested that the susceptibility proneness to coal spontaneous combustion slowly decreased from high to moderate to low with an increase of coalification. The effect of pore structures on spontaneous combustion of coal is important for the current work. Pores are the pathways through which oxygen transports within coal, which determine the amount of oxygen exposed to the coal surface. Karsner and Perlmutter demonstrated that the oxidation rate increased with an increase of gas diffusion rate within coal.
particles. Zhang et al. concluded that the heterogeneity of pore distribution reduced the spontaneous combustion tendency by virtue of the pore size distribution through multiscale and multifractal analyses. The oxidation rate of coal had a significant correlation with the densification on lignite; when the densification increased, the number of active sites on coal surface capable of reacting with oxygen molecules decreased, and in addition, the oxidation rate decreased. The oxidation rate of coal was influenced by the oxygen concentration that reacted with the coal. However, when the oxygen concentration was below a threshold value, the oxidation reaction was inhibited. Therefore, the pore structure affects the reaction rate between coal and oxygen, which consequently affects the tendency of coal spontaneous combustion.

The activity and content of each functional group directly affect the spontaneous combustion tendency of coal. Zhang et al. found that during the spontaneous combustion of coal, —OH had dominant effects on the emanating heat from coal. Tang concluded that the increases in the content of aliphatic hydrocarbon and oxygen-containing functional groups increased the probability of coal spontaneous combustion. Li et al. found that active sites, which were generated from the thermal decomposition of oxygen-containing groups, accelerated the oxidation of coal. Zhong et al. found that the increasing content of the aliphatic hydrocarbon group and hydroxyl group resulted in an accelerated oxidation reaction rate, which was more likely to result in spontaneous combustion. Therefore, different functional groups have different effects on the low-temperature oxidation of coal spontaneous combustion, resulting in different tendency of coal spontaneous combustion.

The moisture content of coal has a complex influence on the spontaneous combustion. Clemens et al. found that moisture could inhibit the production of stabilized radicals and quicken the oxidation of coal. Wu et al. indicated that the mechanism for moisture to influence upon spontaneous combustion changed with the reaction stage.

The inherent properties of coal determine the degree of difficulty in spontaneous combustion. At present, methods that evaluate the spontaneous combustion trend of coal have not been generally accepted. Researchers have proposed numerous research methods to analyze the oxidation rate of coal spontaneous combustion. These include low-temperature oxidation, adiabatic oxidation, thermal gravity analysis, and crossing point temperature methods. Nevertheless, few studies have examined the relationship between multiattribute coupling and spontaneous combustion tendency.

Grey relational analysis was appropriate to resolve the complex interrelationships between multiple factors and research objects. In the past few years, grey relational analysis has been widely used in coal spontaneous combustion for research and prediction. By using grey relational analysis, Wang calculated the grey correlation degree of index gas at different characteristic temperatures, optimized the early prediction index gas of coal spontaneous combustion at different temperature stages, and established perfect index gas systems. Zhang analyzed various functional groups in the infrared spectra of different coal samples by means of grey relational analysis and obtained the quantitative variation law of different functional groups with temperature. The root cause of coal spontaneous combustion was the reaction and exothermic heat between oxygen and functional groups. Therefore, the tendency of coal spontaneous combustion is related to the pore structure, functional groups, and other coal parameters. Based on the grey relational analysis, we try to establish a multiparameter model to quantify the probability for the spontaneous combustion tendency of coal. The cross-point temperature (CPT) is used to measure the spontaneous combustion tendency of coal to verify the accuracy of the model.

The objective of this study was to establish a multiparameter model to comprehensively and systematically analyze the spontaneous combustion tendency of coal. The experiments utilized CPT measurements, cryogenic nitrogen adsorption measurements, and Fourier transform infrared (FTIR) spectroscopy. To effectively eliminate the complicated effect of water during spontaneous combustion, samples were dried in a vacuum oven at 60 °C for 24 h to ensure that the moisture content was approximately consistent. Subsequently, pore structures and functional groups of the samples were obtained. Thereafter, the grey relational grade between the spontaneous combustion tendency and the pore structures and functional groups of coal was analyzed by grey relational analysis. Eventually, a new model describing the coal spontaneous combustion tendency was established by multiple regression analysis.

2. EXPERIMENTS AND METHODS

2.1. Coal Samples. Fresh coal samples were directly collected from coalfields throughout northern China following the Chinese standard (GB/T 19222-2003) and were carefully sealed and transported to the laboratory for experiments. Subsequently, the samples were crushed and screened out with different particle sizes. In accordance with the Chinese standard (GB/T 6948-2008), the vitrinite random reflectance (Rt) of all coal samples on corresponding polished sections was measured with a photometer microscope. Table 1 provides the coal coalfield location and the coal rank of samples in this experiment.

### Table 1. Coal Ranks of the Samples

| samples | coalfield          | Rt (%) | coal rank |
|---------|--------------------|--------|-----------|
| S1      | Huolinhe           | 0.36   | lignite   |
| S2      | Linnancang         | 0.68   | gas coal  |
| S3      | Donghuantu         | 0.74   | gas coal  |
| S4      | Tangshan (7 coal seam) | 0.90 | 1/3 coking coal |
| S5      | Qianjiaying        | 1.24   | coking coal |
| S6      | Xingtai            | 2.21   | meager coal |
| S7      | Yangquan           | 2.51   | anthracite |

2.2. CPT Measurement. This experiment was conducted by the self-developed device based on program heating technology. Samples with a mass of 50 ± 0.1 g and a particle size of 50–80 mesh were placed in the container with a heating rate of 0.8 °C/min, and the temperatures of coal and oven were recorded. From initiation, the container was continuously filled with high-purity nitrogen for 5 min to remove the impurity gas. Then, dry air, instead of high-purity nitrogen, at a flow rate of 96 mL/min was established and then adjusted to 8 mL/min when the coal sample temperature reached 35 °C. When the coal temperature caught up with the oven temperature, samples reached the CPT. In CPT measurements, the spontaneous combustion tendency was described...
by the comprehensive judgment index (CJI). CJI of the coal was calculated by the following eqs \(1-3\).^{5,455}

\[
I_{\phi(O_2)} = \frac{\phi(O_2) - 15.5}{15.5} \times 100
\]

where \(I\) is the CJI; \(\phi(O_2)\) is the oxygen concentration at the outlet of the coal sample in the container when the coal temperature is 70 °C; \(T_{CPT}\) is the CPT; \(I_{\phi(O_2)}\) is the oxygen concentration index at the outlet of the coal sample when the coal temperature is 70 °C; \(I_{CPT}\) is the temperature index of the CPT; \(W_{\phi(O_2)}\) and \(W_{CPT}\) are the weights of low-temperature and rapid oxidation stage, respectively, and their values are 0.6 and 0.4; \(\phi\) is the amplification factor, 40; 300 is the correction factor.

When \(I < 600, 600 < I < 1200,\) and \(I > 1200,\) the tendency of coal spontaneous combustion is easy to spontaneous combustion, spontaneous combustion, and difficult to spontaneous combustion, respectively.

Obtained by experiment and calculation, the CJI and other parameters of the spontaneous combustion tendency are shown in Table 2.

### Table 2. CJI and Other Parameters in the CPT Experiment

| samples | \(\phi(O_2)\) | \(I_{\phi(O_2)}\) | \(T_{CPT}\) | \(I_{CPT}\) | \(I\) |
|---------|---------------|-----------------|-------------|-------------|-----|
| S\(_1\)  | 20.07         | 29.48           | 154.8       | 10.57       | 531.76 |
| S\(_2\)  | 19.83         | 27.94           | 166.1       | 18.57       | 667.59 |
| S\(_3\)  | 20.41         | 31.68           | 178.3       | 27.36       | 873.36 |
| S\(_4\)  | 19.20         | 23.87           | 192.1       | 37.21       | 868.24 |
| S\(_5\)  | 19.06         | 22.97           | 206.0       | 47.14       | 1005.51 |
| S\(_6\)  | 20.70         | 33.55           | 202.3       | 44.50       | 1217.16 |
| S\(_7\)  | 20.73         | 33.74           | 214.2       | 53.00       | 1357.81 |

The Rr of samples in different areas ranged from 0.56 to 2.51 and were obtained by vitrinite random reflectance. It can be concluded from Table 1 that the Rr of the samples increased with increasing metamorphism. The CJI values of the samples were calculated by eqs \(1-3\). The results are displayed in Table 2. The spontaneous combustion tendency of \(S_1\) was easy to spontaneous combustion, of \(S_2, S_3, S_4,\) and \(S_5\) was spontaneous combustion, and of \(S_6\) and \(S_7\) was difficult to spontaneous combustion. The degree of metamorphism was positively correlated with the CJI values.

For analyzing the content of functional groups after peak fitting more intuitively, the representatives of the main functional groups with the most reactivity were selected to calculate the content relative of peak area,\(^{56}\) and the results are shown in Table 4.

### 3. RESULTS AND DISCUSSION

#### 3.1. Experimental Analysis.

The Rr of samples in different areas ranged from 0.56 to 2.51 and were obtained by vitrinite random reflectance. It can be concluded from Table 1 that the Rr of the samples increased with increasing metamorphism. The CJI values of the samples were calculated by eqs \(1-3\). The results are displayed in Table 2. The spontaneous combustion tendency of \(S_1\) was easy to spontaneous combustion, of \(S_2, S_3, S_4,\) and \(S_5\) was spontaneous combustion, and of \(S_6\) and \(S_7\) was difficult to spontaneous combustion. The degree of metamorphism was positively correlated with the CJI of the coal spontaneous combustion tendency. Specifically, the lower the coal rank, the smaller the value of CJI and the stronger the spontaneous combustion tendency. Table 3 shows the pore structure parameters for the cryogenic nitrogen adsorption experiment. The average pore diameter was negatively correlated with the CJI of the coal spontaneous combustion tendency. The correlation between other pore parameters of coal and CJI was not significant. Table 4 shows the peak area content of the main functional groups for the FTIR spectroscopy experiment. The hydroxyl, methyl, methylene, and carbon—carbon double bonds were negatively correlated with the CJI values. The benzene substituent was positively correlated with the CJI values.

However, the spontaneous combustion tendency of coal should be determined by the coupling of multiple factors such as its chemical composition and physical structure. Therefore, it was necessary to comprehensively study the combined effect of the internal composition and structure of coal on the spontaneous combustion tendency. In addition, determining the correlation between each factor and the spontaneous combustion tendency, finding out the key influencing factors, and establishing a multifactor comprehensive prediction model of spontaneous combustion tendency are also necessary.

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**Table 3. Pore Structure Parameters of Coal**

| samples | \(V_1\) cm\(^3\)/g | \(V_2\) cm\(^3\)/g | \(V_3\) cm\(^3\)/g | \(S_{BET}\) m\(^2\)/g | \(D_{av}\) nm | \(V_1\) cm\(^3\)/g |
|---------|------------------|------------------|------------------|-------------------|--------------|------------------|
| \(S_1\) | 0.0030           | 0.0041           | 0.0024           | 4.53              | 12.26        | 0.00949          |
| \(S_2\) | 0.0005           | 0.0002           | 0.0001           | 0.31              | 11.63        | 0.00081          |
| \(S_3\) | 0.0003           | 0.0002           | 0.0001           | 0.47              | 8.01         | 0.00054          |
| \(S_4\) | 0.0027           | 0.0017           | 0.0007           | 0.24              | 7.43         | 0.00012          |
| \(S_5\) | 0.0003           | 0.0002           | 0.0001           | 0.17              | 8.20         | 0.00059          |
| \(S_6\) | 0.0005           | 0.0003           | 0.0002           | 5.18              | 6.22         | 0.00097          |
| \(S_7\) | 0.0030           | 0.0021           | 0.0008           | 3.01              | 6.15         | 0.00598          |

\(^{56}\)Note: \(V_1, V_2,\) and \(V_3\) are the pore volumes of micropores (<1 nm), mesopores (10–50 nm), and macropores (>50 nm), respectively. \(S_{BET}\) is the BET specific surface area; \(D_{av}\) is the average pore diameter; \(V_1\) is the single point adsorption total pore volume.
3.2. Grey Relational Analysis. Grey system theory was initially proposed by Professor Deng in 1982 to solve situations where information was partly available and unavailable. Grey relational analysis was appropriate to resolve the complex interrelationships between multiple factors and research objects. In our study, grey relational analysis was used to determine the complicated relationships between multiple parameters for the spontaneous combustion tendency of coal.

The CJI \( (I) \) was selected to be the reference sequence \( X_0(k) \). The basic parameters of coal samples were selected to be the comparison sequence \( X_i(k) \). The data obtained from the experiments were normalized to ensure that the scatter range of the sequence was small. The maximum method was used for normalization, and the results of \( X_0(k)^* \) and \( X_i(k)^* \) are shown in Table 5. Grey relational coefficients for normalized data were computed using eqs 4–7:

\[
\Delta_i(k) = |X_0(k)^* - X_i(k)^*| \\
\Delta_{max} = \max_{i} \max_{k} |X_0(k)^* - X_i(k)^*| \\
\Delta_{min} = \min_{i} \min_{k} |X_0(k)^* - X_i(k)^*| \\
R_i(k) = \frac{\Delta_{min} + q\Delta_{max}}{\Delta_i(k) + q\Delta_{max}}
\]

where \( k \) is the number of coal samples; \( i \) is the number of parameters; \( X_0(k)^* \) is the normalized reference sequence; \( X_i(k)^* \) is the normalized comparative sequence. \( \Delta_i(k) \) is the deviation sequence of the reference sequence and compara-
Figure 4. Peak-fitting FTIR figure of $S_3$.

Figure 5. Peak-fitting FTIR figure of $S_4$.

Figure 6. Peak-fitting FTIR figure of $S_5$.

Figure 7. Peak-fitting FTIR figure of $S_6$. 
Using eq 8 to average the grey relational coefficients, the results are displayed in Table 6. The grey relational grade is the most moderate when $X_i(k)$ is the macropore parameter; $X_i(k)$ is the mesopore parameter; $X_i(k)$ is the micropore parameter; $X_i(k)$ is the parameter of the single point adsorption total pore volume; $X_i(k)$ is the parameter of the BET specific surface area; $X_i(k)$ is the parameter of the average pore diameter; $X_i(k)$ is the parameter of the hydroxyl content; $X_i(k)$ is the parameter of the methyl and methylene contents; $X_i(k)$ is the parameter of the carboxyl content; $X_i(k)$ is the parameter of the aromatic hydrogen content; $X_i(k)$ is the parameter of the carbon—carbon double bond content; finally, $X_i(k)$ is the parameter of the benzene substituent content.

Table 6. Grey Relational Grade between Each Parameter and CJI

| parameters | $X_1(k)$ | $X_2(k)$ | $X_3(k)$ | $X_4(k)$ | $X_5(k)$ | $X_6(k)$ | $X_7(k)$ | $X_8(k)$ | $X_9(k)$ | $X_{10}(k)$ | $X_{11}(k)$ | $X_{12}(k)$ |
|------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|-----------|-----------|-----------|
| $\gamma$   | 0.5368  | 0.4436  | 0.4169  | 0.4914  | 0.4924  | 0.6566  | 0.6370  | 0.6693  | 0.5914  | 0.5942    | 0.5449    | 0.8642    |

where $m$ is the experimental number of coal samples. $\gamma$ is the integral grey relational grade.

As shown in Table 6, macropores ($X_6(k)$) with a value of 0.4169 and benzene substituent ($X_{12}(k)$) with a value of 0.8642 are the minimum and maximum grey relational grades, respectively. The greater the grey relational grade value, the better the represented relationship between each parameter and CJI. The parameter effects and the optimal level of each parameter can be determined on the basis of grey relational grade.

In terms of physical structure, the pore diameter was highly correlated with the CJI of spontaneous combustion tendency. Agnieszka suggested that the spontaneous combustion tendency decreased with the decrease of the macropore diameter. With the deepening of the degree of coalification, the
pore diameter decreased, while the macropores decreased and the mesopores developed. The gas flow in the pore changed from laminar permeability to molecular diffusion. The gas flow capacity weakened, which reduced the tendency of coal spontaneous combustion.

In terms of molecular composition, the functional groups, benzene substituent, hydroxyl groups, methyl groups, and methylene groups, were highly correlated with CJI for spontaneous combustion tendency. The essence of coal oxidation was the stretching vibration and bending vibration of the functional groups. Zhong suggested that the content of the oxygen functional group and the aliphatic hydrocarbon group affects the tendency of coal spontaneous combustion. Hydrogen on methyl and methylene initially reacted with oxygen to produce carbon-free radicals, while the methyl and methylene that provided hydrogen react with hydroxyl groups on the oxygen functional groups to produce water and a large methylene that provided hydrogen react with hydroxyl groups to produce carbon-free radicals, while the methyl and methylene groups, were highly correlated with CJI for spontaneous combustion tendency. The essence of coal spontaneous combustion. The gas effects the tendency of coal spontaneous combustion. In terms of molecular composition, the functional groups, hydroxyl, methyl, methylene, and benzene substituent of seven grades between each factor and CJI of coal spontaneous combustion. The gas effects the tendency of coal spontaneous combustion. Therefore, parameters quantifying the average pore diameter, the regression equation must be verified by statistical test of the results.

As one may observe in Table 8, all four variables requested entered the model, and none was eliminated.

Table 7. Multiple Regression Variable Data of Samples

| samples | Y | X1 | X2 | X3 | X4 |
|---------|---|----|----|----|----|
| S1      | 531.76 | 12.26 | 0.1968 | 0.0552 | 0.0270 |
| S2      | 667.59 | 11.63 | 0.1767 | 0.0376 | 0.0301 |
| S3      | 873.36 | 8.01 | 0.1753 | 0.0355 | 0.0285 |
| S4      | 868.24 | 7.43 | 0.1656 | 0.0350 | 0.0312 |
| S5      | 1005.51 | 8.20 | 0.1624 | 0.0298 | 0.0336 |
| S6      | 1217.16 | 6.22 | 0.1537 | 0.0332 | 0.0374 |
| S7      | 1357.81 | 6.15 | 0.1525 | 0.0410 | 0.0465 |

The dependent variable is Y, the explained variable; X is the explaining variables; β is the regression coefficient; ε is the random error.

Table 8. Input/Removed Variable

| variables entered | variables removed | method |
|-------------------|-------------------|--------|
| X1, X2, X3, X4    | none              | enter  |

The determination coefficient represents the fitting effectiveness of the model to accurately summarize the data. To verify the fitting goodness of the model, the determination coefficient should be examined. The closer the determination coefficient was to 1, the more accurate the fitting effect was. According to the data in Table 9, the determination coefficient R is 0.989; R square is 0.978, and adjusted R square is 0.933. All these parameters were closer to 1 at high values, indicating that the regression equation had a high degree of fitting accuracy.

As shown in Table 10, the value of F was 22.011, and the given significance level of α was 0.05. Obtaining a value for F from a test threshold table, F_{0.05} (4, 2) = 19.247, it is evident that F > F_{0.05}(k, n-k-1)(k is the number of parameters; n is the number of coal samples). The significance level shown in Table 9 was 0.044 less than 0.05. This indicates that the model was statistically significant. Consequently, the above indicated that the linear relationship of the model was significantly established at the confidence level.
According to the data in Table 11, the $t$ values of the four explaining variables ($X_1$, $X_2$, $X_3$, and $X_4$) obtained were $|t_1| = 1.832$, $|t_2| = 0.53$, $|t_3| = 0.191$, and $|t_4| = 2.268$, respectively. The given significance level of $\alpha$ was 0.05, and the degree of freedom (df) was 2 ($n-k-1 = 2$). When $t_{0.025}(2) = 6.205$ was calculated, it can be observed that the values of all four variables were less than the critical value; therefore, the null hypothesis was rejected. In other words, the four explaining variables introduced in the model all had significant influence under the level. All explaining variables passed the significance test of variables.

The collinearity diagnosis of the model was validated by data in Table 11. The variance inflation factors (VIFs) of the four explaining variables were all less than 10, indicating that the model did not contain multicollinearity problem.

The normal P–P plot of the regression standardized residual is the relationship between the accumulative proportion of normal variables and the accumulative proportion of normal distribution. In Figure 9, the predicted points are distributed on both sides of the line without significant deviation, which indicate that the random variables were well-described by the normal distribution, and the residual distribution is also approximately normal.

In conclusion, the model satisfied the significance test with high reliability, and the variables were randomly distributed and independent. The model passed the regression coefficient and residual analysis test, and the regression equation was statistically significant. In summary, we determined the multifactor prediction model of coal spontaneous combustion tendency as follows

$$Y = 1176.737 - 52.79X_1 - 3290.746X_2 + 1228.511X_3 + 21582.536X_4$$

To verify the practicability of the model, fresh coal samples from Tangshan mine (8 coal seam) and Chengde mine were selected. According to the same experimental operation, corresponding experimental data of coal spontaneous combustion tendency and influencing factors are obtained, as shown in Table 12.

The experimental data obtained from coal samples and used for verification were substituted into the formula for the multifactor prediction model of spontaneous combustion tendency. The actual and predicted CJI values of coal spontaneous combustion tendency were calculated, as shown in Table 13.

By calculating the CJI for the coal seam spontaneous combustion tendency, both coal mine (8 coal seam) and Chengde mine demonstrate a tendency for spontaneous combustion. By comparing the predicted value and the experimental value, the relative errors of two coal samples of the model were 1.42 and 4.25%, respectively. These small relative errors verified the reasonableness and validity of the prediction model.

4. CONCLUSIONS

In this study, the influence of multiple parameter coupling on the tendency of coal spontaneous combustion was studied.

By the measure of vitrinite random reflectance, the Rr of each coal sample increased with an increasing metamorphism degree. Meanwhile, the CJI of coal spontaneous combustion tendency increased with Rr.

According to grey relational analysis, the grey relational grades between CJI and the parameters of coal samples were...
obtained. The grey relational grade between each parameter and CJI was in the descending order: benzene substituent, methyl, methylene, average pore diameter, hydroxyl, aromatic hydrogen, carboxyl, carbon—carbon double bond, micropores, BET specific surface area, single point adsorption total pore volume, mesopores, and macropores. Among these parameters, the benzene substituent had the maximum grey relational grade of 0.8642 and carboxyl had the minimum grey relational grade, 0.4169.

Based on the results from the SPSS Statistics software for regression fitting, the prediction model was established. The R squared value of model was 0.978. The significance level, the F-distribution, the t-distribution, the collinearity diagnosis, and the residual distribution of the model satisfied all verification requirements. In addition, two coal samples were selected to verify the model to compare the measured values and predicted values of the multiple regression equation. The relative errors for CJI found in this verification were 1.42 and 4.25%, respectively. This suggests that the multiple regression model had higher prediction accuracy and relatively smaller error ranges. This results in an improvement in the application of predicting the spontaneous combustion tendency of coal.

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### Notes

The authors declare no competing financial interest.

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