

1 Thermal properties of coal during low temperature oxidation using  
2 a grey correlation method

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11 A B S T R A C T

12 The low temperature oxidation of coal is a contradictory and unified dynamic process of coexisting  
13 mass and heat transfer. The thermophysical properties are crucial during coal spontaneous  
14 combustion. In the current paper, the variations of moisture, ash, volatiles, fixed carbon and  
15 thermophysical properties (thermal diffusivity, specific heat and thermal conductivity) of three coal  
16 samples from 30 °C to 300 °C were studied, and their grey correlation was analyzed. The results  
17 indicated that with the increase of temperature, the free moisture of Coals A and B decreased first  
18 but then increased, while the free moisture of Coal C kept decreasing without a later increase. The  
19 variation of surface moisture was consistent with that of free moisture. The trend of volatiles and  
20 fixed carbon was completely the opposite, showing a significant negative correlation. Ash was less  
21 affected by temperature. Along with the rise of temperature, the thermal diffusivity of three coal

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1 samples decreased first but later increased, and the specific heat was always in a state of increasing.  
2 The change in thermal conductivity was mainly affected by specific heat. By calculating the gray  
3 correlation degree, the major factors affecting the thermophysical properties were obtained.

4 *Keywords:*

5 Heat transfer

6 Coal spontaneous combustion

7 Moisture

8 Thermal conductivity

9 Grey correlation

<b>Nomenclature</b>			
$X_i(k)$	$k_{\text{th}}$ factor in the $i_{\text{th}}$ sequence	$r_i$	correlation degree of the $i_{\text{th}}$ comparison sequence
$x_i(k)$	dimensionless value of $X_i(k)$		
$n$	number of sequences	$M$	average molar mass (g/mol)
$m$	number of factors in the sequence	$R$	molar gas constant (8.314 J/(mol K))
$\xi_i(k)$	grey correlation coefficient of the $k_{\text{th}}$ factor in the $i_{\text{th}}$ sequence		Abbreviation
$x_0(k)$	dimensionless value of the $k_{\text{th}}$ factor of the reference sequence	TD	thermal diffusivity (mm <sup>2</sup> /s)
		SH	specific heat (10 <sup>3</sup> J/(kg K))
$\rho$	a resolution coefficient ranging from 0–1, usually taking $\rho = 0.5$	TC	thermal conductivity (W/(m K))

## 2 1. Introduction

3 Spontaneous combustion of coal accompanies with most coal mining processes [1,2] leading to  
 4 coal fire, which causes a persistent and serious hazard [3] to the mining process: life loss of mine  
 5 workers, machinery damage and stoppage of further mining. Almost all major coal-producing  
 6 countries (USA, Australia, China, South Africa, and India) have reported coal fire disasters [4–7],  
 7 which cause huge waste of energy resources and pose a serious threat to the environment, human  
 8 health and safety [8,9]. Low temperature oxidation of coal is the most important roots causing its  
 9 spontaneous combustion. When coal comes in contact with oxygen, low temperature oxidation of  
 10 coal always occurs, whether the coal is being mined, or being left naturally and unprocessed in a  
 11 coal pile, or even during transportation. Such low temperature oxidation processes are extremely  
 12 complicated involving physicochemical adsorption and oxidation reactions [10], and has therefore  
 13 attracted much attention from the perspectives of safety, resources and the environment.

14 Wang et al. [11] analyzed the CO and CO<sub>2</sub> production rates in oxidation and desorption  
 15 experiments by gas chromatography, and explained the low temperature oxidation process of coal

1 by proposing a multiple reaction mechanism. Li et al. [12] comparatively analyzed the heat release  
2 rate of low temperature oxidation process of coal determined by various methods, and proposed a  
3 method based on the thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC)  
4 to determine the low temperature oxidation kinetics of coal. Zhao et al. [13] studied the self-heating  
5 characteristics of dry coal samples, and analyzed the effects of gas flow rate, particle size and  
6 moisture content on the low temperature oxidation process of coal. Arisoy et al. [14] analyzed the  
7 coal oxidation kinetics data and explained the changes of kinetics in the low temperature region by  
8 deriving a new rate equation model.

9 Wang et al. [15] investigated the oxygen consumption characteristics of coal and oxidation  
10 products, and revealed the mechanism of low temperature oxidation of coal. Chen et al. [16]  
11 comparatively analyzed the thermochemical and kinetic characteristics of individual coal and mixed  
12 coal samples, and obtained their difference in low temperature oxidation. Zhang et al. [17] studied  
13 the dynamics and thermodynamics of low temperature oxidation process of coal based on the  
14 changes of elements, and discussed the mechanism of spontaneous combustion of coal. Itay et al.  
15 [18] measured the low temperature oxidation rate of coal, and found that the reaction of coal with  
16 oxygen is the main source of exotherm. Wang et al. [19] explored the variation of reactive  
17 functional groups in five coal samples (brown coal, gas coal, fat coal, and anthracite) during low  
18 temperature oxidation by using adiabatic oxidation tests, Fourier transform infrared (FTIR) and  
19 temperature programmed experiments. Kaji et al. [20] researched the low temperature oxidation of  
20 five different metamorphic coals in the temperature range of 30–250 °C, and found that  
21 oxygen-containing functional groups play an important role in the low temperature oxidation  
22 process of coal.

23 The spontaneous combustion process of coal is essentially an unsteady heat and mass transfer

1 process involving multiple internal heat sources. Low temperature oxidation of coal is an  
2 irreversible reaction process involving extremely complex mechanisms, and its essence is to slowly  
3 absorb oxygen from the environment, oxidize and release heat, causing coal to gradually accelerate  
4 oxidation [16]. Low temperature oxidation of coal spans a wide range of temperatures (from room  
5 temperature to ca. 300 °C) [12,21,22]. When the heat generated by oxidation accumulates to such  
6 an extent that heat cannot be dissipated in time, the temperature will gradually rise and eventually  
7 lead to spontaneous combustion of coal. The heat transfer characteristics of coal is the major factor  
8 affecting such heat dissipation. Therefore, studying the thermal characteristics of coal oxidation  
9 process can help to understand the heat generation and dissipation characteristics of coal  
10 spontaneous combustion process and provide a theoretical basis to prevention of spontaneous  
11 combustion. The thermal conductivity (TC), specific heat (SH) and thermal diffusivity (TD) of coal  
12 are different in temperature sensitivity under different atmospheres [23–25]. The variation of SH  
13 with temperature is usually contrary to that of TD with temperature [26,27]. There are large  
14 differences in the thermophysical properties of coal with different metamorphic grades [28]. The  
15 thermophysical properties of coal are affected by many factors [29]. However, most researchers  
16 only qualitatively analyzed the relationship between these influencing factors and thermophysical  
17 parameters, with very few studies showing a quantitative analysis which is important to study the  
18 oxidation of coal. Therefore, the purpose of the current study is to: (1) analyze the change of  
19 proximate analysis indexes (volatiles, moisture, fixed carbon, and ash) in coal in a temperature  
20 range of 30–300 °C, (2) investigate the variation of TD, SH, and TC of three coals with temperature,  
21 (3) determine the major influencing factors affecting the thermal properties of coal through the gray  
22 correlation analysis. The thermal properties of coal are extremely important attributes affecting  
23 spontaneous combustion, with changes in its intrinsic composition leading to large differences in

1 thermal properties. Thus, the main focus of the current paper is to analyze the quantitative  
2 relationship between coal thermophysical parameters and its internal components through a grey  
3 correlation method, and to reveal the inherent causes of heat changes during low temperature  
4 oxidation.

## 5 **2. Materials and methodology**

### 6 *2.1 Coal samples*

7 Bituminous coal is the most widely distributed and abundant coal in nature. It is used in a wide  
8 range of applications, such as boiler fuels, raw materials for the modern chemical industry, and civil  
9 fuels. Due to these characteristics, the proportion of bituminous coal spontaneous combustion is  
10 relatively large. Therefore, three different metamorphic levels of bituminous coal (Coal A, Coal B,  
11 and Coal C) were selected as research objects. Coal A, Coal B, and Coal C were taken from the  
12 coalmines of Aiweier, Liuhuanguo, and Sangshuping, respectively. To prevent oxidation of the  
13 coal samples, the collected coal samples were immediately wrapped with fresh films. Before the  
14 experiment, all the coal sample were first stripped of their oxide layers on the surfaces, and then  
15 pulverized into a powder having a particle size of 140–160 mesh. Such prepared coal samples were  
16 stored in dry sealed bags for later tests.

### 17 *2.2 Experiments on thermophysical parameters*

18 The apparatus used in the experiment was a laser-flash apparatus LFA 457 (Netzsch GmbH,  
19 Selb, Germany), the details of which were described by Min et al. [30]. The powdered coal samples  
20 were processed into tablets. To accommodate the size of the sample holder and prevent heat loss,  
21 the diameter and thickness of the coal tablets were made to 12.7 mm and 1.0 mm, respectively. The  
22 tablets were placed in the testing apparatus through the sample holder, and tested at an air flow rate  
23 of 100 mL/min. Due to thermal inertia, a large heating rate would cause the coal sample to exceed

1 the set temperature, resulting in irreversible changes in the coal molecular structure [23]. Therefore,  
2 in order to ensure the stability and reliability of the experimental results, the heating rate was set to  
3 1 °C/min. The temperature measurement covered the range of 30–300 °C, and a test point was set  
4 for every 30 °C increment. Each coal tablet was tested three times at the set collection point, using  
5 the average of three measurements as the thermophysical parameters for each temperature point  
6 [31].

### 7 2.3 Proximate analysis experiment

8 The proximate analysis indexes of coal were less sensitive to temperature in the range of 30–  
9 300 °C. When the oxidation treatment temperature interval was small, the difference in the  
10 proximate analysis indexes of coal was insignificant. Therefore, a larger temperature gradient was  
11 selected to oxidize the coal samples. Each selected coal samples was divided into 5 groups, where  
12 coal samples were separately heated from room temperature to 90, 150, 210, 270, and 300 °C at  
13 1 °C/min heating rate by a temperature programming device. Dry air was used as the purge gas, and  
14 the flow rate was set to 100 mL/min. The treated coal samples were approximately analyzed by an  
15 automatic industrial analyzer, which provided the content of fixed carbon, ash, moisture and  
16 volatiles in the coal samples [32,33]. The results of the proximate analysis of the raw coal samples  
17 were presented in Table 1.

## 18 Table 1

## 19 3. Results and discussion

### 20 3.1 Variation of proximate analysis indexes

#### 21 3.1.1 Moisture

22 As shown in Fig. 1, the change in capillary moisture of Coal C and Coal A before 270 °C was  
23 small, but that of Coal B was large. With rising temperature, the surface moisture of Coal A and

1 Coal B initially went down but then went up; that of Coal C gradually decreased first, then slightly  
2 increased, and finally declined. The free moisture curve showed that before 150 °C, the free  
3 moisture of Coal A and Coal B gradually decreased with increasing temperature, and then gradually  
4 increased after 150 °C. The free moisture of Coal C gradually decreased before 210 °C, slightly  
5 increased in the temperature range of 210–270 °C, and decreased again over 250 °C. The moisture  
6 in coal is composed of free moisture and bound moisture [34,35]. Free moisture refers to the water  
7 adsorbed on the outer surface and into the internal pores of coal, which is combined with coal  
8 physically not chemically. The free moisture further includes the capillary moisture adsorbed in the  
9 capillary pores inside the coal particles and the surface moisture adsorbed on the surface of the coal  
10 particles. The surface moisture was directly evaporated from the outer surface of the coal, and the  
11 capillary moisture needed to be transported to the surface by capillary action for evaporation [36].  
12 Surface moisture was more likely to evaporate than capillary moisture. Therefore, the capillary  
13 moisture content of the coal sample was smaller than the surface moisture. The coal sample mainly  
14 underwent a physical reaction before 150 °C. With the rising temperature, the water evaporated  
15 gradually, causing a reduction in the free water content. After 150 °C, the carboxyl group, carbonyl  
16 group, phenolic group and aliphatic hydrogen in the coal were decomposed to produce moisture  
17 [37,38], and the coal reacted with oxygen in the air to generate moisture. This caused the free  
18 moisture of Coals A and B to increase with increasing temperature, and that of the Coal C to  
19 decrease slowly and then gradually increase in the range from 150 to 270 °C. After 270 °C, the rate  
20 of water evaporation was greater than that of water production, causing a prompt decrease of free  
21 moisture of Coal C.

22 **Fig. 1**

23 *3.1.2 Ash, volatiles, and fixed carbon*



1 From Fig. 2, the variation of volatiles with temperature was completely opposite to that of  
2 fixed carbon, and their curves were in a symmetrical form except for Coal B. Before 90 °C, due to  
3 the lower temperature, coal and oxygen hardly reacted chemically, and the molecular structure of  
4 coal did not decompose, so the volatiles changed little with temperature. The volatiles were mainly  
5 pyrolysis products of organic matter, including gases generated by the cracking of various small  
6 molecular structures in coal. The volatiles of Coals A and B gradually decreased in the temperature  
7 range of 90–210 °C, and began to rise after 210 °C. The explanation for this trend was as follows.  
8 Before 210 °C, some functional groups (methoxy, hydroxyl, and phenolic groups) in the coal  
9 reacted with oxygen to form H<sub>2</sub>O, CO, and CO<sub>2</sub> as the oxidation temperature increased. At the same  
10 time, the bridging bonds, alkyl side chains, and other molecules in the coal were cleaved to produce  
11 small molecular structures to volatilize out during the oxidation [39]. The oxidized coal samples  
12 had less active components on the surface and formed a stable structure containing carboxyl or  
13 carbonyl group [40,41], resulting in a decrease in volatiles generated during the pyrolysis. When the  
14 oxidation temperature exceeded 210 °C, the cyclic macromolecular structure which was stable at  
15 low temperature in coal was decomposed and reacted with oxygen to form unsaturated  
16 hydrocarbons. These small molecular hydrocarbons produced alkane gas during pyrolysis, which  
17 led to the gradual increase of volatiles. The volatiles change of Coals A and B was opposite to that  
18 of Coal C, indicating that the molecular structure in Coal C was more reactive with oxygen than the  
19 other two. During the reaction between coal and oxygen, a large number of small volatile molecular  
20 structures were formed, leading to the gradual increase of volatiles before 270 °C, which was  
21 consistent with the research by Fredericks [42]. Volatiles and fixed carbon content can be used as  
22 the basis for coal metamorphism [43–45]. As the degree of metamorphism deepened, the content of  
23 volatiles gradually decreased, and that of fixed carbon gradually increased. The variation of

1 volatiles and fixed carbon with oxidation temperature further indicated that oxidation would affect  
2 the degree of coal metamorphism. Organic matter was the main component of coal. The sum of the  
3 mass fractions of volatiles and fixed carbon in coal samples could approximately represent the total  
4 mass fraction of organic matter. Therefore, the volatiles content was opposite to the fixed carbon  
5 content. It is remarkable from [Table 2](#) that the change of ash content of three coal samples was  
6 insensitive to the oxidation temperature. The ash in coal was derived from minerals which were  
7 mainly composed of muscovite, dolomite, quartz, pyrite, calcite, and kaolinite [\[46\]](#). In the low  
8 temperature oxidation process, minerals mainly acted as catalysts [\[47\]](#), and underwent a series of  
9 physical and chemical reactions during the combustion process [\[48\]](#). Therefore, the ash change was  
10 small within the temperature range of 30–300 °C.

11 **Fig. 2**

12 **Table 2**

### 13 *3.2 Variation of thermophysical parameters*

14 It is noticeable in [Figs. 3 and 4](#) that with rising temperature, TD of three coals went down first  
15 but then up in the temperature range of 240–300 °C. SH gradually increased with temperature, but  
16 the rate of increase decreased. Coal was an amorphous disordered solid material composed of a  
17 large number of different molecules, containing amorphous, crystals (calcite, quartz, kaolinite, and  
18 mica) and other impurities. Vibration modes in disordered materials included extendons and locons.  
19 Locons were localized and non-propagating, and had no significant contribution to heat transfer  
20 [\[49\]](#). Therefore, heat transfer in coal was mainly dependent on extendons. Extendons contained two  
21 modes of propagation: propagons and diffusons. Propagons were low-frequency propagation modes  
22 that transfer energy through phonons, while diffusons acted as a localized mode of transferring heat  
23 through diffusion [\[50,51\]](#) as the name suggests. At lower temperatures, the propagons propagation

1 mode dominated, and heat propagated through the phonons eventually reaching a temperature  
2 equilibrium. As the temperature increased, the number of phonons and collisions between phonons  
3 increased, resulting in a decrease in the mean free path and the lifetime of phonons [52]. Therefore,  
4 TD gradually decreased with increasing temperature. With further increasing temperature, the  
5 oxidation reaction of coal gradually increased, causing the increase of coal disorder. The  
6 contribution of the diffusons mode to heat transfer was gradually increased, and heat was further  
7 propagated by diffusion. Therefore, TD decreased slowly until it increased.

8 **Fig. 3**

9 **Fig. 4**

10 SH represents the potential of a material to absorb and retain heat that is primarily stored by  
11 exciting a free mode of vibration in the structure of the material [31]. Below 300 °C, the effect of  
12 temperature on SH could be explained by the solid molecular thermal theory of Einstein and Debye.  
13 Due to the relatively small mass of carbon atoms and the strong binding force in the crystal lattice,  
14 the lattice vibration excitation was extremely large within the temperature range of 30–300 °C [53].  
15 As temperature rose, the kinetic energy of coal molecules was gradually enhanced by absorbing  
16 energy, thus the molecules became more active and therefore the degree of freedom of vibration  
17 increased. The increase in SH with temperature was attributed to the increase in the degree of  
18 freedom of vibration [54]. With rising temperature, the oxygen-containing groups, side chains and  
19 other small molecular structures in the coal molecular structure began to crack, and the oxidation  
20 reaction of coal was therefore enhanced causing the increase of active structures in coal. The  
21 transformation of molecular structure might have released additional vibration modes [55], so the  
22 SH was always increasing. Since the absorption of energy by coal molecules was a gradual  
23 weakening process, the total energy in the coal sample gradually reached a saturated state, so SH

1 increase rate gradually decreased. As the chemical reaction between coal and oxygen was further  
2 enhanced, the molecular structure of coal underwent irreversible changes, resulting in the decrease  
3 of SH in the high temperature region.

4 The variation of TC of Coals A and B was consistent. With the temperature rising constantly,  
5 their TC first increased, then reduced, and finally rose again. TC of Coal C was always increasing.  
6 Neglecting the change in density, TC varied with the product of TD and SH [56,57]. Before 120 °C,  
7 the decreasing rate of TD decreased gradually, while the increase of SH offset the decrease of TC  
8 caused by the decrease of TD. Therefore, TC of Coals A and B gradually increased. After 120 °C,  
9 the influence of TD on TC was gradually increased, so TC was slightly reduced. With the further  
10 increase of temperature, TD began to increase gradually after decreasing to the minimal value.  
11 Under the influence of SH and TD, TC increased again. TC of Coal C was more affected by SH  
12 than by TD. It can be seen from the overall change that TC of three coal samples was more  
13 correlated with SH than TD. From a microscopic point of view, since the temperature characteristics  
14 of TD and SH were responded to various types of vibration states with temperature changes, the  
15 behavior of TC had the same origin [58]. Therefore, TC was affected by phonon scattering and  
16 vibrational freedom, and the change of TC was the result of the interaction between the two.

### 17 3.3 Grey correlation analysis

18 The changes of thermophysical parameters were influenced by moisture, ash, volatiles, and  
19 fixed carbon [59]. For moisture, it gradually evaporated with increasing temperature, resulting in  
20 the increase of coal porosity [60]. The originally filled moisture in the pores of coal was gradually  
21 replaced by air. The thermophysical properties of the moisture were greatly different from that of  
22 the air, which caused changes in the thermophysical properties of the coal. Ash was mainly derived  
23 from various minerals in coal, and the difference among the thermophysical properties of each

1 mineral was also responsible for the change in the thermophysical properties of coal. The change in  
 2 volatiles and fixed carbon represented a change in the molecular structure of the coal, which was an  
 3 intrinsic cause of the difference in thermal properties. To obtain the main factors affecting the  
 4 thermal properties of coal, the correlation between the proximate analysis indexes and the  
 5 thermophysical parameters was analyzed according to the grey correlation degree theory [61]. The  
 6 TD, SH, and TC were used as the reference sequence, while the moisture, ash, volatiles, and fixed  
 7 carbon were used as the comparison sequence. Due to the different dimensions of the factors in  
 8 each sequence, comparisons between different sequences could not be made. Therefore, in order to  
 9 ensure the reliability of the result, the reference and comparison sequences were dimensionlessly  
 10 processed using Eq. (1).

$$x_i(k) = \frac{X_i(k)}{\frac{1}{m} \sum_{k=1}^m X_i(k)}, (i = 0, 1, \dots, n; k = 1, 2, \dots, m) \quad (1)$$

12 After the dimensionless processing, the correlation coefficient was calculated by Eq. (2), as shown  
 13 in Fig. 5.

$$\xi_i(k) = \frac{\min_i \min_k |x_0(k) - x_i(k)| + \rho \max_i \max_k |x_0(k) - x_i(k)|}{|x_0(k) - x_i(k)| + \rho \max_i \max_k |x_0(k) - x_i(k)|} \quad (2)$$

15 **Fig. 5**

16 From Fig. 5, the correlation between the moisture at different temperatures and thermophysical  
 17 parameters of the three coal samples was relatively low, while the correlation among ash, volatiles,  
 18 fixed carbon, and thermophysical parameters was higher than that of moisture, which also showed a  
 19 phasic characteristics. Therefore, the following analysis was focused on the relationship between  
 20 three indicators (ash, volatiles, and fixed carbon) of proximate analysis with multiple  
 21 thermophysical parameters. For Coal A, as the temperature increased, the correlation between the  
 22 three indicators and TD increased first, then decreased, and finally increased again. The correlation

1 between the three indicators with SH and TC increased first and then decreased. The correlation of  
 2 the thermophysical parameters of Coal B basically showed a trend of initial increase and subsequent  
 3 decrease. For Coal C, the change law of the correlation of TD was insignificant, and the correlation  
 4 between the three indexes and SH, TC increased first but decreased subsequently. The correlation  
 5 degree between the reference sequence and the comparison sequence at each temperature was called  
 6 the correlation coefficient [62]. Because the number of information was excessively scattered, the  
 7 overall comparison could not be performed. Thus, the degree of correlation between the comparison  
 8 sequence and the reference sequence was obtained by Eq. (3). The grey correlation degree was  
 9 displayed in Table 3.

$$r_i = \frac{1}{m} \sum_{k=1}^m \xi_i(k), (i = 1, 2, \dots, n) \quad (3)$$

### 11 Table 3

12 It is noted in Table 3 that moisture, ash, volatiles, and fixed carbon had different correlations  
 13 with thermophysical parameters. The major influencing factors of TD of the three coals were  
 14 volatiles, ash, and fixed carbon, respectively. For the same coal sample, the major influencing  
 15 factors of SH were the same as that of TC. The change of fixed carbon had the greatest influence on  
 16 SH and TC of coal A. The main influencing factors to SH and TC of Coals B and C were volatiles.  
 17 TD represented the ability of the sample to be locally disturbed by temperature to reach equilibrium.  
 18 Coal was of a highly heterogeneous mixture with extremely complex chemical structure. There  
 19 were great differences in the characteristics of coal samples in different mining areas, so the factors  
 20 influencing TD were rather different. From Fig. 3, both TC and SH showed an increasing tendency  
 21 as the temperature rose. The change of the two was consistent and showed a strong correlation,  
 22 which was why the major factors affecting the SH and TC of coal sample were chime with the same  
 23 one. With rising of temperature, the increase in SH gradually became slower, and SH even

1 decreased in high temperature region. This was because the average molar mass  $M$  gradually  
2 increased with the release of volatiles, resulting in a decrease in the  $3R/M$  value, thus lowering the  
3 SH [63]. Herrin et al. found that TC of bituminous coal was inversely proportional to the sum of  
4 carbon and volatiles content [59]. Furthermore, it can be seen from the results of section 3.2 that the  
5 thermophysical properties of coal were related to vibration and propagation modes which were  
6 significantly impacted by the coal molecular structure. These further explained why SH and TC  
7 were major affected by volatiles and fixed carbon.

#### 8 **4. Conclusions**

9 In the current paper, the variations of moisture, ash, volatiles, fixed carbon, and  
10 thermophysical parameters of three coals at the range of 30–300 °C were studied and the correlation  
11 among them was analyzed. With increasing temperature, the free moisture of Coals A and B  
12 decreased first but then increased, while the free moisture of Coal C showed a continuous  
13 downward trend. Compared with capillary water, the overall change of surface moisture was  
14 consistent with that of free moisture. With the increasing temperature, the changes in volatiles of the  
15 three coals were inversely correlated with the change of fixed carbon. The ash in coal was derived  
16 from minerals and varied little with increasing oxidation temperature. TD decreased at first but then  
17 increased with increasing temperature. SH gradually increased with temperature, but its rate of  
18 increase decreased. With increasing temperature, TC of Coal C was always increasing. The  
19 variation of TC of Coals A and B was the same: first increased and then decreased. The overall  
20 trend of thermophysical parameters showed that TC of the three coals was more correlated with SH.  
21 Through the gray correlation analysis, the quantitative relationship between the proximate analysis  
22 indexes and the thermophysical parameters was established, and the main factors affecting the  
23 thermophysical properties were obtained. For the same coal sample, the main factors affecting SH

1 and TC were the same. The main influencing factors to SH and TC of three coal samples were  
2 concentrated approximately on two main analytical indicators: volatiles and fixed carbon. In  
3 summary, through the above analysis method combining qualitative and quantitative, it was finally  
4 found that the change of molecular structure inside coal was the main factor affecting  
5 thermophysical properties, further revealing the mechanism of low temperature oxidation heat  
6 transfer of coal.

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- 1 **List of tables**
- 2 **Table 1**
- 3 Proximate analysis of three raw coal samples (air-dried basis, mass%).
- 4 **Table 2**
- 5 Variation of ash corresponding to temperatures for three coal samples.
- 6 **Table 3**
- 7 Grey correlation degree of three coals.

1 **Table 1**

2 Proximate analysis of three raw coal samples (air-dried basis, mass%).

Specimen	Moisture	Ash	Volatiles	Fixed carbon
Coal A	0.18	9.34	21.58	68.90
Coal B	0.67	30.80	12.19	56.34
Coal C	1.74	8.47	24.87	64.92



1 **Table 2**

2 Variation of ash corresponding to temperatures for three coal samples.

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Specimen	Ash (%)						Maximum variation rate
	30 °C	90 °C	150 °C	210 °C	270 °C	300 °C	
Coal A	9.34	9.16	9.10	9.06	8.73	8.96	6.63 %
Coal B	30.80	30.99	30.63	30.04	30.02	29.95	2.76 %
Coal C	8.47	8.83	8.72	8.43	8.57	9.07	7.08 %

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3

1 **Table 3**

2 Grey correlation degree of three coals.

Specimen	Thermophysical parameters	Grey relational grade			
		Moisture	Ash	Volatile	Fixed carbon
Coal A	Thermal diffusivity	0.5421	0.8986	0.9022	0.8764
	Specific heat	0.5400	0.7601	0.7534	0.7802
	Thermal conductivity	0.5120	0.8977	0.9057	0.9275
Coal B	Thermal diffusivity	0.5430	0.6656	0.6133	0.6376
	Specific heat	0.4926	0.6772	0.7301	0.7012
	Thermal conductivity	0.4965	0.8547	0.8996	0.8730
Coal C	Thermal diffusivity	0.5730	0.7251	0.6300	0.7725
	Specific heat	0.4697	0.6585	0.7400	0.6407
	Thermal conductivity	0.4898	0.7221	0.8397	0.7027

3

1 **Figure captions**

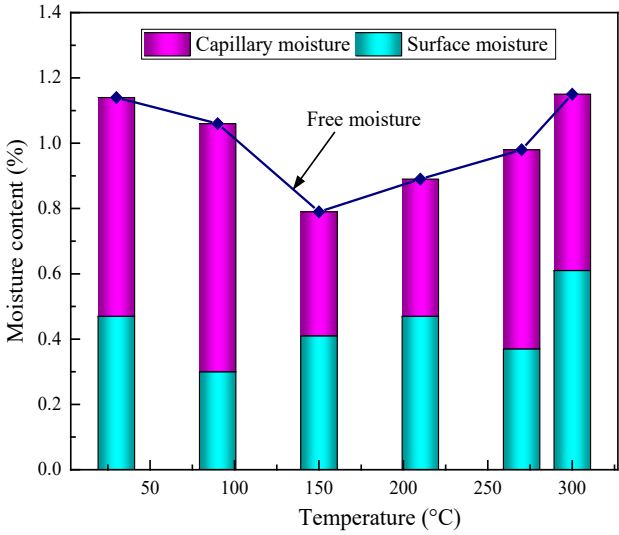
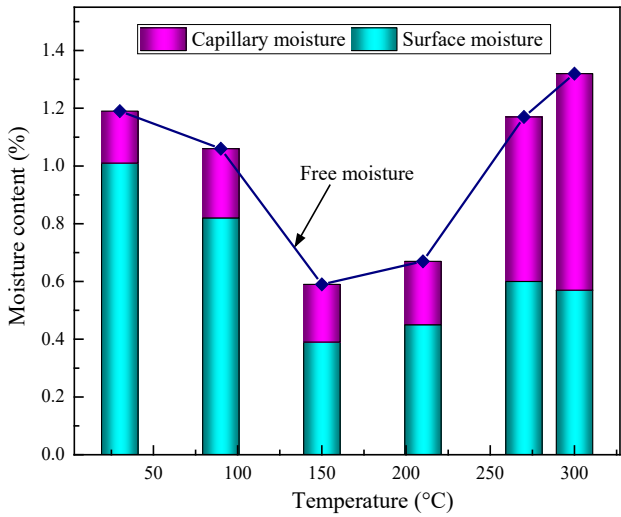
2 **Fig. 1.** Change in moisture content of three coals at corresponding temperatures.

3 **Fig. 2.** Change in volatiles and fixed carbon of three coals at corresponding temperatures.

4 **Fig. 3.** Temperature dependence of thermophysical parameters for coal samples.

5 **Fig. 4.** Rate of variation for the thermophysical parameters of coal samples.

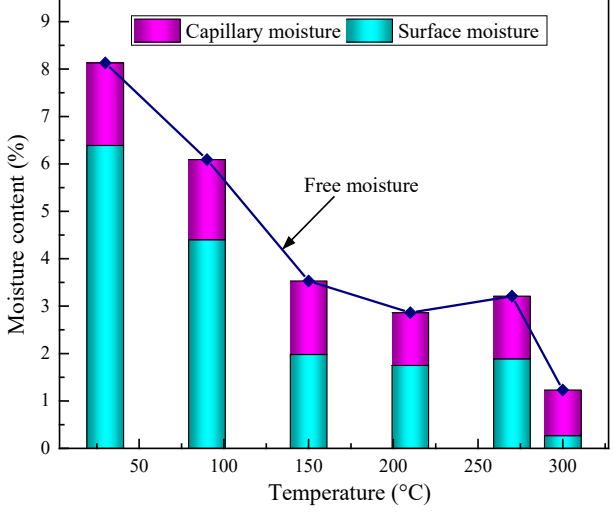
6 **Fig. 5.** Correlation coefficient between thermophysical parameters and proximate analysis indexes  
7 of coal samples.



1  
2

Coal A

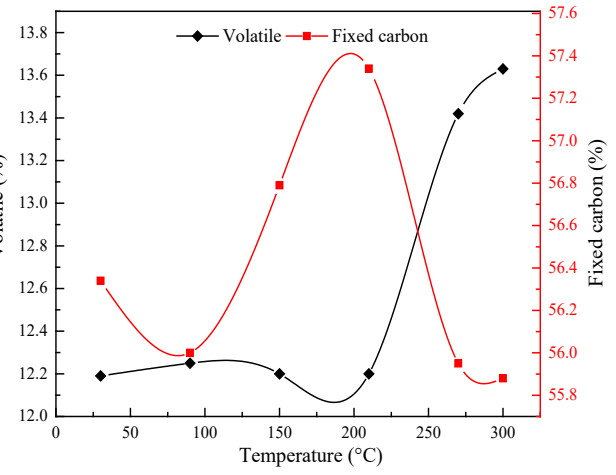
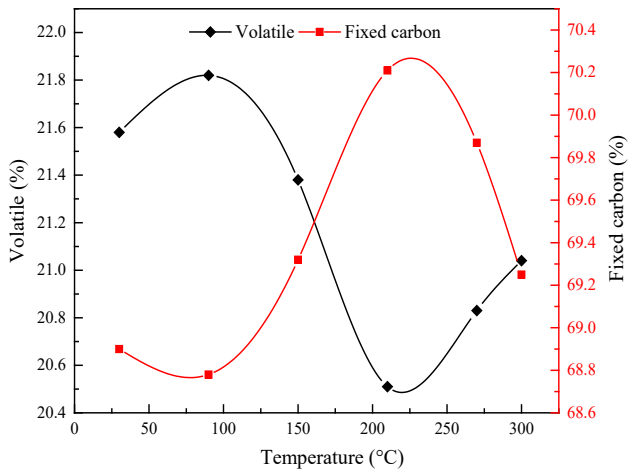
Coal B



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Coal C

5 **Fig. 1.** Change in moisture content of three coals at corresponding temperatures.

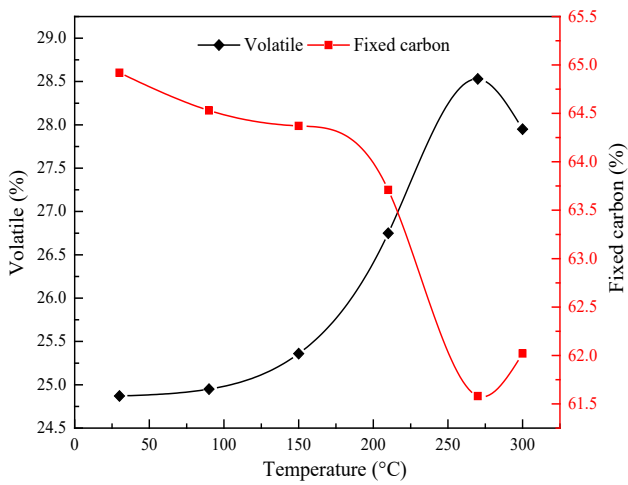


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Coal A

Coal B

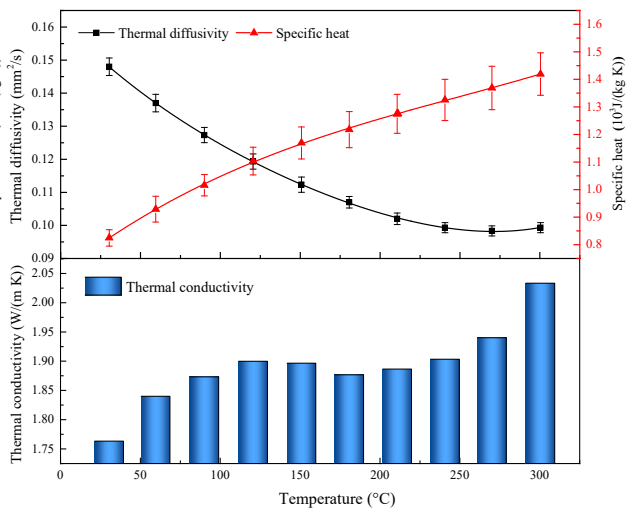
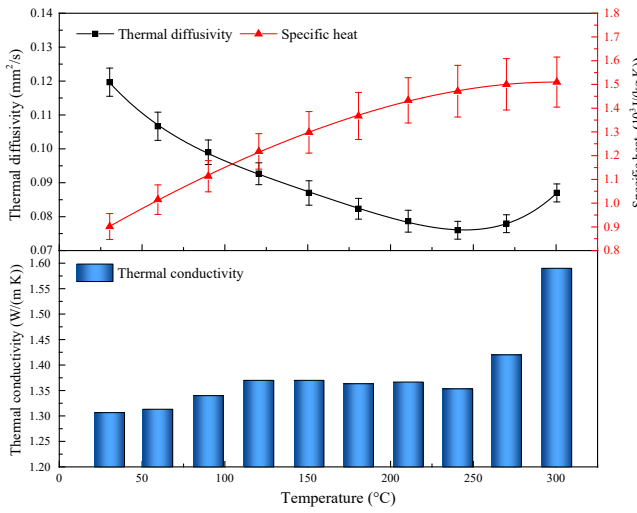


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Coal C

5 **Fig. 2.** Change in volatiles and fixed carbon of three coals at corresponding temperatures.

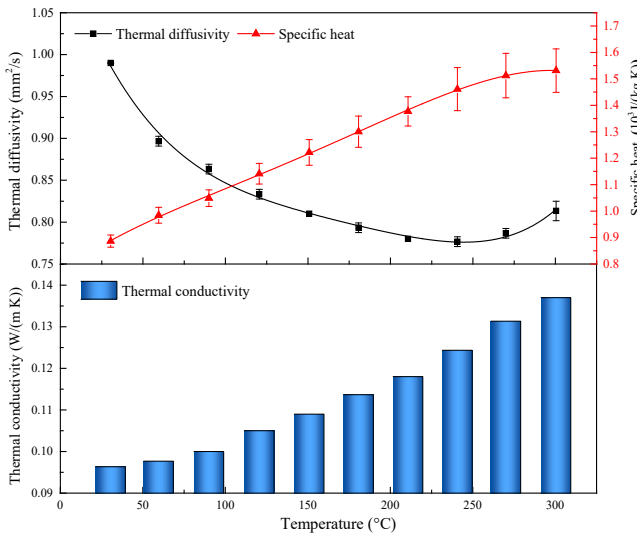


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Coal A

Coal B

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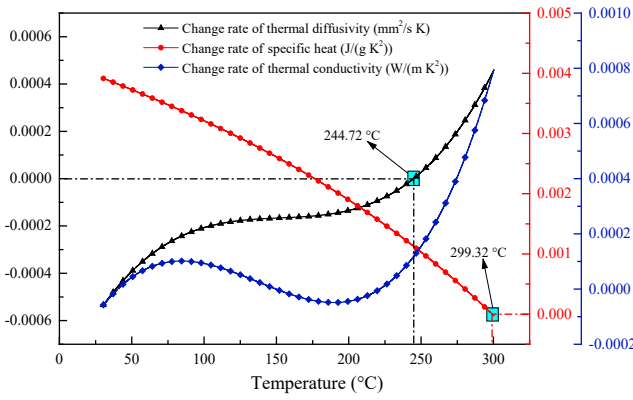


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Coal C

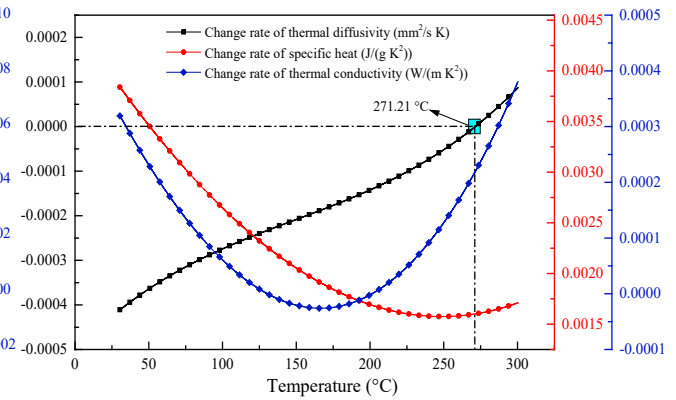
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5 **Fig. 3.** Temperature dependence of thermophysical parameters for coal samples.



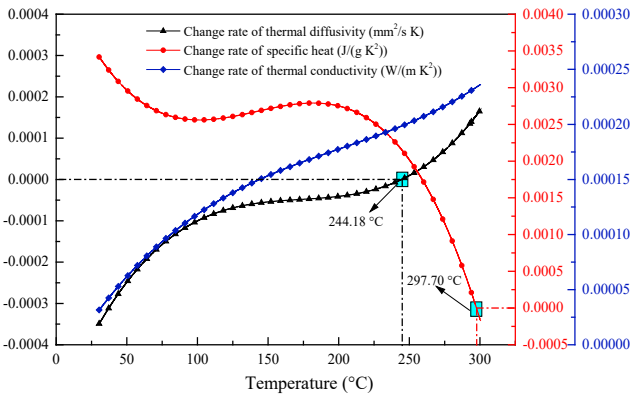
1

Coal A



2

Coal B

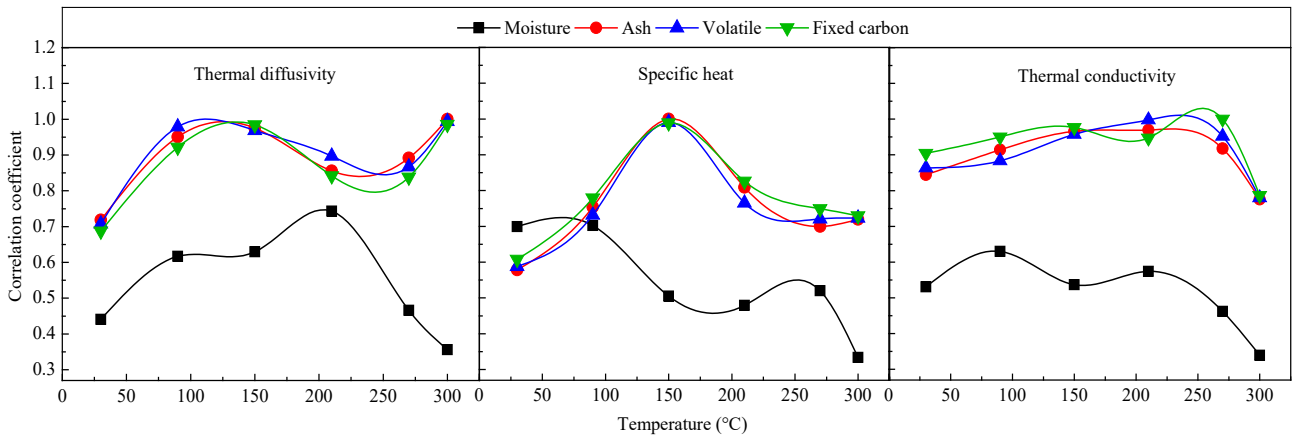


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Coal C

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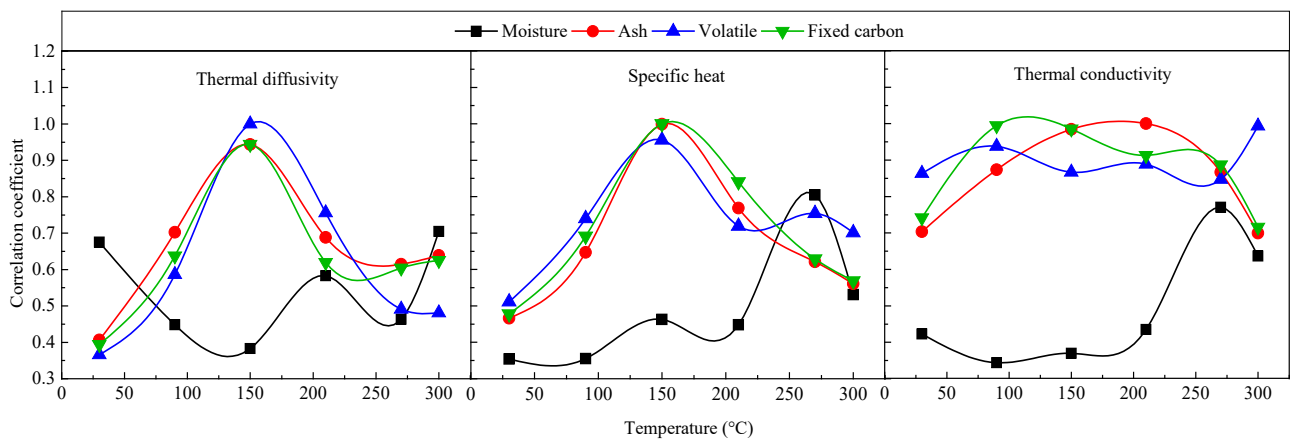
5 **Fig. 4.** Rate of variation for the thermophysical parameters of coal samples.



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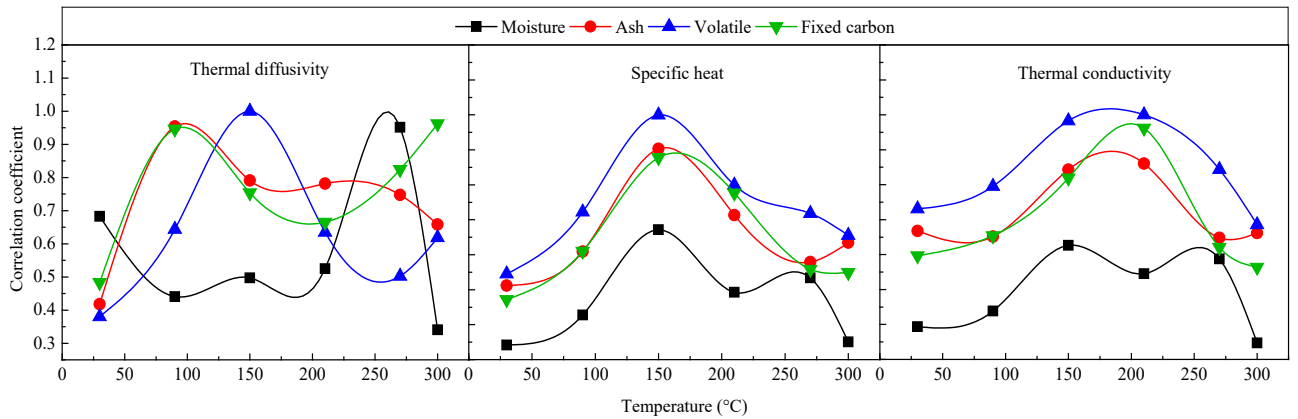
Coal A



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Coal B



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Coal C

7 **Fig. 5.** Correlation coefficient between thermophysical parameters and proximate analysis indexes  
 8 of coal samples.

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