Effects of Moisture on the Ignition and Combustion Characteristics of Lignite Particles: Modeling and Experimental Study

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ABSTRACT: The influence of the moisture content on the ignition and combustion characteristics of lignite single particles was studied using an ignition model of single coal particles with moisture and experimental investigations in a visual drop tube furnace under the temperature of 1300 K. The moisture content and the lignite particle size were varied within the ranges of 0–20% and 75–250 μm, respectively. The images of the combustion process illustrated that higher moisture content caused a significant ignition delay. The probability of homogeneous ignition was greatest when the particle size was 125–150 μm and the moisture content was 5%. An ignition model was employed to explain the mechanism of the influence of moisture content on the ignition and combustion characteristics, which embedded the chemical percolation devolatilization model to increase the accuracy of predictions. The predicted results show that there was an overlap in the release of moisture and volatile matter from the lignite particle during the combustion at a high heating rate. The devolatilization rate increases with the increase of moisture, which explains the increase in the probability of homogeneous ignition and fragmentation. Both particle size and moisture content have two-sided effects on the ignition mode, which causes the complexity and irregularity of the ignition mode of particles with moisture.

1. INTRODUCTION

With the rapid growth in the economy and an increase in energy requirement, coal is still the dominant energy resource. The combustion of lignite has gradually attracted attention because it is low-grade coal with the advantages of low mining cost, rich reserves, high content of volatile matter, and low amount of pollution-forming elements. However, the utilization of lignite is limited due to its disadvantage of high moisture content and low calorific value. The moisture content of lignite in China is generally 25–40%, while the moisture content of lignite mined in Australia’s Latrobe valley can be as high as 55–70%. Therefore, lignite is generally dried before combustion, but the conventional hot-dry processes cannot guarantee the complete removal of moisture in coals.

Moisture may change the combustion characteristics of coal. Tahmasebi et al. studied the effects of moisture content on ignition and combustion behavior of Chinese and Indonesian lignite particles with the particle size in the range of 75–105 μm at temperatures of 400–550 °C. The results showed that the ignition delays increased by 83 and 160 ms when the moisture contents were 10 and 20%, respectively. In addition, high moisture content leads to an increase in fragmentation. Clemems et al. suggested that the moisture content did not affect the diffusion of oxygen to the functional group on the surface of coal when the coal contained 5–10% moisture at low temperatures, whereas the increase in moisture content accelerated the formation of peroxide. Zhai et al. studied the effect of moisture immersion on active functional groups and characteristic temperatures of bituminous coal. The results revealed that soaked coals were more prone to spontaneous combustion than raw coal because of changes in the number of functional groups and characteristic temperature. It is generally believed that moisture is released completely from coal particles before devolatilization and has no effect on its ignition mode. Pratinoaoa et al. studied the combustion process of Victoria lignite with particle size in the range of 63–104 μm and moisture content of 30% using a flat flame burner reactor and modeling. The results showed that only 10% of moisture was distilled before devolatilization. Therefore, the ignition mode of coal can be changed due to the moisture in pulverized coal particles. However, there are rare reports about the influence of moisture on ignition mode, and the problem only focuses on particle size, heating rate, coal rank, and ambient temperature.

In this study, the primary objective was to understand the effects of moisture content on the combustion characteristics of lignite particles using a visual drop tube furnace, such as ignition mode, ignition delay time, burnout time, and
combustion fragmentation of lignite with different particle sizes through experimental study. Simultaneously, an ignition model of a single particle with moisture was used to analyze the influence mechanism of moisture content on ignition mode.

2. RESULTS AND DISCUSSION

2.1. Effect of Moisture Content on Ignition and Combustion Behavior. To explore the influence of moisture content on ignition and combustion characteristics of lignite particles, the combustion behavior of samples with different moisture contents and particle sizes at 1300 K was recorded, as shown in Figure 1. A pulverized coal particle can occur via either gas-phase combustion of the released VM (homogeneous ignition mode) or heterogeneous ignition of the particle surface (heterogeneous ignition mode). It is observed that the samples with a particle size of 75–90 μm have a higher probability of undergoing a homogeneous ignition mode than the dry samples with particle sizes smaller than 150 μm, and the probability decreases when the particle size is above 200 μm. Therefore, moisture content has a very important influence on the ignition mode of particles, and there are optimum values for the particle size and moisture content.

At the same time, it is found that the characteristics of homogeneous combustion flame of the samples with moisture are different from those of dry samples. The flame of volatile combustion is mostly of a regular spherical shape, whereas the outer edge of the flame is light blue. The reason is that the release of moisture and volatile matter increases the buoyancy and weakens the convective intensity of pulverized coal particles, resulting in the flame taking a regular spherical shape. On the other hand, the char and moisture reaction increases the release of CO and H₂ (C + H₂O = CO + H₂ + 131.85 kJ/kg). Therefore, the volatile matter can burn in a short distance. Meanwhile, the moisture may lead to the increase in oxygen-containing functional groups and oxygen atoms so that the combustible gas can maintain the dynamic combustion state and the outer edge of the flame becomes light blue.

It is worth noticing that all of the particles of different sizes with moisture are broken during combustion. Moisture leads to fragmentations during the combustion of particles, while the dry particles do not break when the particle size is in the range of 200–250 μm. Therefore, higher moisture contents are found to lead to a higher possibility of fragmentation.

The study found that due to the individual differences of particles, various ignition modes can coexist under the same experimental conditions. Figure 2 shows that the proportion of particles in each ignition mode is statistically analyzed by the photos obtained from the visual drop tube furnace (VDTF). The various ignition modes in samples with moisture are more obvious. Therefore, moisture increases the diversity and
The particle with a size below 150 μm increases the possibility of homogeneous ignition due to the presence of moisture. However, the increase in moisture content or the particle size does not increase the rate of homogeneous or hetero-homogeneous ignition. The probability of gas-phase ignition of particles with a moisture content of 5% and particle size of 125–150 μm is the highest, and the ignition mode is transformed from homogeneous to hetero-homogeneous ignition with an increase in moisture content from 5 to 10%.

2.2. Effect of Moisture Content on the Characteristic Time of Combustion. The ignition delay is a critical parameter to distinguish the reactivity of coal. The ignition delay of particles in the visual drop tube furnace (VDTF) can be recorded by a high-speed camera. The average ignition delay time of more than 40 particles under each experimental condition was counted. The average ignition delays of the samples are recorded in Figure 3. Figure 3 illustrates that the ignition delay increases with the increase of moisture content. Meanwhile, the moisture content has a more obvious effect on the ignition delay of large particles. When the particle size is 200–250 μm, the ignition delays of particles with moisture contents of 10 and 20% are 15 and 45 ms, respectively. However, the ignition delay of particles with moisture contents of 5 and 10% is very close to those of dry particles of lignite for the particle size of 75–90 μm. Therefore, the fluctuations in moisture content have almost no effect on ignition delay when the particle size is below 90 μm and the moisture content is less than 10%.

Figure 3. Effect of particle size and moisture content on ignition delay from VDTF experience.

The VDTF experimental results show that the possibility of homogeneous ignition increases due to the moisture in the lignite particle. To explore the influencing mechanism of moisture on the ignition and combustion characteristics, the combustion process of lignite particles with different moisture contents is simulated using the ignition model of single coal particles with moisture. Figure 5 shows the simulation results of the combustion process of lignite particles with different moisture contents and the particle size of 125 μm at 1300 K. Figure 5a shows the effects of moisture on the curves of particle heating and the release of volatile matter. The heating rates of particles and the release rate of the volatile matter in the initial stage decreased with the increase in moisture content, which is due to the gasification latent heat required for the evaporation of moisture. Therefore, the particle ignition delay increased with the increase of moisture content. Figure 5b shows the rate of release of moisture and volatile matter. It is observed that there is an overlapping of moisture and volatile release curves. The moisture release overlaps with the volatile matter and accounts for 1.25 and 3.7% of volatile matter and moisture, respectively. It illustrates that the higher the moisture content, the higher the initial release concentration of volatiles. Hence, the particle with higher moisture content has a higher possibility of homogeneous ignition. On the other hand, the increase in moisture content promotes the release of volatile matter. It can be seen from the energy conservation that the higher the moisture content, the greater the rate of heat loss of moisture, which increases the temperature difference between the particles and the surrounding environment and increases the rate of radiation heat and convective heat transfer rate provided to the particles by the environment. This is in turn due to the acceleration of the particle heating rate during the release of volatile matter. The concentrated release of volatile matter explains the increase of homogeneous ignition and fragmentation during the combustion of lignite particles with moisture. Although the increase in moisture content promoted the concentrated release of volatiles, it is a factor conducive to the occurrence of homogeneous ignition while reducing the release of volatile matter, which is disadvantageous to homogeneous ignition. Therefore, there is an optimal moisture content for homogeneous ignition.

2.3. Mechanism of the Influence of Moisture Content on the Ignition and Combustion of Particle. 2.3.1. Influence of Moisture Content on the Ignition. The VDTF experiments show that the possibility of homogeneous ignition increases due to the moisture in the lignite particle. To explore the influencing mechanism of moisture on the ignition and combustion characteristics, the combustion process of lignite particles with different moisture contents is simulated using the ignition model of single coal particles with moisture. Figure 5 shows the simulation results of the combustion process of lignite particles with different moisture contents and the particle size of 125 μm at 1300 K. Figure 5a shows the effects of moisture on the curves of particle heating and the release of volatile matter. The heating rates of particles and the release rate of the volatile matter in the initial stage decreased with the increase in moisture content, which is due to the gasification latent heat required for the evaporation of moisture. Therefore, the particle ignition delay increased with the increase of moisture content. Figure 5b shows the rate of release of moisture and volatile matter. It is observed that there is an overlapping of moisture and volatile release curves. The moisture release overlaps with the volatile matter and accounts for 1.25 and 3.7% of volatile matter and moisture, respectively. It illustrates that the higher the moisture content, the higher the initial release concentration of volatiles. Hence, the particle with higher moisture content has a higher possibility of homogeneous ignition. On the other hand, the increase in moisture content promotes the release of volatile matter. It can be seen from the energy conservation that the higher the moisture content, the greater the rate of heat loss of moisture, which increases the temperature difference between the particles and the surrounding environment and increases the rate of radiation heat and convective heat transfer rate provided to the particles by the environment. This is in turn due to the acceleration of the particle heating rate during the release of volatile matter. The concentrated release of volatile matter explains the increase of homogeneous ignition and fragmentation during the combustion of lignite particles with moisture. Although the increase in moisture content promoted the concentrated release of volatiles, it is a factor conducive to the occurrence of homogeneous ignition while reducing the release of volatile matter, which is disadvantageous to homogeneous ignition. Therefore, there is an optimal moisture content for homogeneous ignition.

2.3.2. Effect of Moisture Content on the Ignition Characteristics of Particles of Different Sizes. The VDTF
experimental results show that the influence of moisture content on ignition and combustion characteristics of lignite particles of different sizes is very obvious. The experimental results show that the proportion of homogeneous ignition within the particle size range of 125–150 \( \mu \text{m} \) is the largest under different moisture contents. To analyze the influence of the coupling effect of moisture content and particle size on the ignition characteristics, the combustion process of lignite particles with moisture contents of 5 and 20\% and particle sizes of 75 and 200 \( \mu \text{m} \) is simulated, as shown in Figure 6. Figure 6a shows the heating rate of the particles under different conditions. It shows that moisture has only a slight effect on the heating rate of smaller particles, which reveals the reason why moisture has little effect on the ignition delay of particles of small size. Figure 6b shows the release rates of moisture and volatile matter. As shown in Figure 6b, for the particles with moisture content and size of 5\% and 75 \( \mu \text{m} \), 20\% and 75 \( \mu \text{m} \), 5\% and 200 \( \mu \text{m} \), and 20\% and 200 \( \mu \text{m} \), the moisture release overlaps with the volatile matter and accounts for 0.9\% (1.7 \times 10^{-12} \text{ kg}) , 2.4\% (4.56 \times 10^{-12} \text{ kg}) , 0.6\% (2.17 \times 10^{-11} \text{ kg}) , and 0.8\% (2.9 \times 10^{-11} \text{ kg}) of the total volatile matter, respectively. Increasing the moisture increases the overlapping release of moisture and volatiles, especially for smaller particles. Reducing the particle size increases the heating rate, but the amount of volatile matter released is small, and the proportion of overlapped moisture and volatile matter is high, especially at a high moisture content. It reveals the mechanism that moisture significantly affects the ignition mode of smaller particles (as shown in Figure 2). Increasing the particle size can increase the release of volatile matter, which is conducive to the homogeneous ignition of coal particles. The proportion of the homogeneous ignition mode increases with the increase of the particle size for dry pulverized coal particles. However, this characteristic does not appear in the experimental results of particles with moisture. To reveal the reasons, the temperature difference between the center and surface of the particles with different particle sizes and moisture contents are simulated. Figure 7 shows the temperature difference of the particles when the average temperature of the particles is 373 K. The results indicate that the temperature difference increases with the increase of the particle size and moisture content. Therefore, the central moisture release rate of large-sized particles lags behind the average release rate, due to which the moisture of large-sized particles has a greater impact on the initial release of volatile matter. On the other hand, the central moisture that cannot be released quickly may block the voids of coal particles, thereby inhibiting the release of volatiles. Therefore, compared with
dry pulverized coal, moisture reduces the probability of homogeneous ignition of larger particles. The particle size has two sides to the homogeneous ignition of the lignite particle with moisture. Therefore, the ignition mode is determined by the coupling of moisture and particle size and has an optimal particle size for homogeneous ignition mode.

3. CONCLUSIONS
In this paper, the visual experiment and simulation were used to study the effect of moisture content on combustion characteristics. The following conclusions are drawn.

The moisture increases the complexity and diversity of the ignition mode of lignite particles. The probability of homogeneous ignition does not increase with the increasing particle size, which is different from the dry coal particles. The probability of homogeneous ignition is greatest when the particle size is 125−150 µm and the moisture content is 5%.

The effect of volatile pyrolysis and volatile combustion heat on particle heating can be more effectively predicted when the chemical percolation devolatilization (CPD) model is embedded in the ignition model of a single particle with moisture.

Moisture promotes the concentrated release of volatiles, while the increase of moisture reduces the initial release concentration of volatiles (the volatiles released by overlapping with moisture account for 1.25 and 3.7% of the total volatiles, and when the moisture content is 5 and 20%, respectively). The moisture content and particle size have a two-sided effect on the ignition mode of the particle with moisture.

4. MATERIALS AND METHODS

4.1. Sample Preparation. Lignite produced in China was used in the present study. The results from the proximate analysis (ad%) were as follows: \( \text{FC}_{\text{ad}} = 34.27\% \); \( \text{V}_{\text{ad}} = 39.76\% \); \( \text{M}_{\text{ad}} = 21.41\% \); \( \text{A}_{\text{ad}} = 4.56\% \). The results from the ultimate analysis (daf%) were as follows: \( \text{C}_{\text{daf}} = 65.82\% \); \( \text{H}_{\text{daf}} = 4.51\% \); \( \text{O}_{\text{daf}} = 28.78\% \); \( \text{N}_{\text{daf}} = 0.89\% \). To explore the influence of moisture content on ignition and combustion characteristics of samples with different particle sizes, the lignite was separately crushed and sieved to 75−90, 125−150, and 200−250 µm, and they were dried to achieve the moisture contents of 20, 10, 5, and 0%, respectively. The preparation process of particles with different moisture contents is as follows: (i) the samples (1 ± 0.1 g) with different particle sizes were dried in a drying oven on forced convection at the temperature of 105 °C until the weight became constant and the moisture content was calculated as received base (\( M_i \)); (ii) the sample of each particle size was divided into 20 equal parts with a mass of 1 ± 0.1 g, and they were also dried at 105 °C; and (iii) a sample was taken out every 2 min, and the rate of moisture content was calculated according to eq 1. The moisture loss curve of the three particle sizes is shown in Figure 8. Finally, the

\[
M_i = M_{\text{ar}} - \frac{m_i - m_0}{m_0} \times 100\%
\]

where \( M_i \) is the moisture content of the sample at time \( i \) (%), \( m_i \) is the mass of the sample before drying (kg), and \( m_0 \) is the mass of the sample at time \( 0 \) (kg).

4.2. Experimental Apparatus and Conditions. The schematic of the ignition and combustion rig of lignite particles used in the current study is shown in Figure 9. The visual drop tube furnace (VDTF) was composed of a reactor, a furnace, a feeding system, an air supply system, a smoke exhaust, and a dust removal system. The reactor was a vertical quartz reactor with an inner diameter of 50 mm and a length of 1000 mm. The reactor was evenly heated by the surrounding heating wires to ensure the uniform distribution of temperature. The samples with the moisture content of 20, 10, 5, and 0% (error of less than ± 0.5%) were prepared by adjusting the residence time according to the moisture loss curve.
effective reaction area of pulverized coal particles was 650 mm from the outlet of the feeder to the upper end of the lower water cooler. A fluidized-bed coal feeder was used to feed the samples to the reactor through a water-cooled injector at a rate of 0.1 g/min with a flow rate of 200 mL/min when the furnace temperature was 1300 K. At this temperature, the highest heating rate of particles was estimated to be $10^4$ K/s. The difference between the set and measured temperature was within 2%. The fluidization feed method guaranteed the high discrete of particles in VDTF. A high-speed camera with a shutter rate of 1300 FPS/s and visual resolution of 1280 × 1024 pixels was used to record the combustion of coal particles through 30 mm × 600 mm observation windows.

4.3. Ignition Model of Single Coal Particle with Moisture. 4.3.1. Model Development. An ignition model of a single coal particle with moisture was used to obtain the parameters of the combustion process and determine the dominant mechanism of moisture on the ignition and combustion characteristics. The illustration of the proposed ignition model is shown in Figure 10. The model assumed that

- The inside of the particle was considered to be isotropic, and the radiation cloud was composed of regular spheres.

4.3.2. Conservation Equations. The model of the single coal particle with moisture maintained energy and mass conservations during the simulation process.

Particle mass consisted of three parts: moisture, volatile matter, and char.

$$\frac{dm_p}{dt} = \frac{dm_C}{dt} + \frac{dm_{VM}}{dt} + \frac{dm_M}{dt} \quad (2)$$

where $m_p$ is the mass of particles (kg), $m_C$ is the mass of char (kg), $m_{VM}$ is the mass of volatile matter (kg), and $m_M$ is the mass of moisture (kg).

Energy balance was controlled by the rates of radiation and convection heat exchange between the ambient atmosphere and the particles, the internal heating process, the rate of heat loss of evaporation of moisture and devolatilization, and the rate of heat generation of char combustion, as given by eq 3.

$$m_p \frac{dT_i}{dt} = \dot{Q}_C - \dot{Q}_{cond} - \dot{Q}_{conv} - \dot{Q}_{rad} - \dot{Q}_M - \dot{Q}_{VM} \quad (3)$$

where $\dot{Q}_C$ is the rate of the heat of chemical reaction (J/s), $\dot{Q}_{cond}$ is the rate of conduction heat from a particle’s surface to its core (J/s), $\dot{Q}_{conv}$ is the convection heat rate of the particle and ambient atmosphere (J/s), $\dot{Q}_{rad}$ is the radiation heat rate (J/s), $\dot{Q}_M$ is the heat loss rate due to the evaporation of moisture (J/s), $\dot{Q}_{VM}$ is the heat loss rate due to evaporation of devolatilization (J/s), $T_i$ is the surface temperature of the particle (K), and $\dot{c}_p$ is the specific heat of the particle (J/kg/K).

The value of $\dot{Q}_{conv}$ can be calculated using eq 4.

$$\dot{Q}_{conv} = h(T_s - T_p)(\pi d_p^2) = \frac{Nu\lambda}{d_p}(T_p - T_s) \quad (4)$$

where $T_s$ is the ambient gas temperature (K), $d_p$ is the particle diameter (m), $h$ is the convection coefficient (W/m²/K) calculated using the correlation of $Nu\lambda/d_p$, and $\lambda$ is the conductivity coefficient of gas (W/m/K).

Particle internal thermal conductive process is calculated for the unsteady state and coupled with the Biot number $Bi$

$$\dot{Q}_{cond} = \frac{\lambda_p}{d_p}(T_s - T_C)(\pi d_p^2) \quad (5)$$

here

$$Bi = \frac{T_s - T_C}{T_s - T_g} = \frac{\delta/\lambda_p A}{1/hA} = \frac{\delta h d_p}{\lambda_p} \quad (6)$$

The temperature of the particle’s core can be calculated using eq 7.

$$T_C = T_s - Bi(T_s - T_g) \quad (7)$$

where $T_C$ is the center temperature of the particle (K), $\lambda_p$ is the conduction coefficient of the particle (J/s/K/cm), and $Bi$ is the ratio of the conductive resistance to convective resistance of the particle and has quite a small value ($Bi < 0.1$) for small dry particle ($d < 200 \mu m$). However, internal heat conduction has a more significant influence on the combustion process of the wet pulverized coal particle than that of the dry particles. Moreover, $\delta$ is the characteristic length of the sphere.
The rate of radiation heat transfer $Q_{rad}$ can be calculated without volatile combustion using eq 8.

$$Q_{rad} = \sigma e (T_i^4 - T_S^4) \left(\frac{dT_i}{dt}\right)$$

(8)

$$T_i = \frac{3(m_{VM,i} - m_{VM,i-1}) \times h_{VM}}{4\pi(d_i^4 - d_{i-1}^4) \times c_{pi,i} \times \rho_i}$$

(9)

where $T_i$ is the radiant cloud temperature (K), $h_{VM}$ is the heat of volatile combustion (kJ/kg), $d_i$ is the radius of radiant cloud, which is generally not more than 5 times the particle size, $m_{cpi,i}$ is the specific heat of combustion products (J/kg/K), and $\rho_i$ is the density of combustion products (kg/m$^3$).

The heat of volatile combustion can be calculated based on the pyrolysis component yield as predicted by the CPD model.

$$h_{VM} = \sum_i \frac{Q_{tar} \times m_{tar,i} + Q_{CH_4} \times m_{CH_4,i} + Q_{CO} \times m_{CO,i}}{m_{VM,i} \times n}$$

(10)

where $m_{tar}$, $m_{CH_4}$, and $m_{CO}$ are the masses of tar, CH$_4$, and CO produced during unit mass coal pyrolysis, respectively (g), and $Q_{tar}$ (37.5 kJ/g), $Q_{CH_4}$ (10.1 kJ/g), and $Q_{CO}$ (55.8 kJ/g) are the calorific values of tar, CH$_4$, and CO, respectively.

The rate of heat loss from the evaporation of moisture $\dot{Q}_M$ can be calculated without volatile combustion using eq 11.

$$\dot{Q}_M = r_M \Delta h_M = \frac{dM_{VM}}{dt} \Delta h_M$$

(11)

where $r_M$ is the rate of moisture evaporation (kg/s) and $\Delta h_M$ is the heat loss due to the evaporation of moisture (kJ/kg), whereas $\Delta h_M = 2400$ kJ/kg.\(^{25}\)

The heat loss rate of devolatilization $\dot{Q}_{VM}$ is calculated using eq 12.

$$\dot{Q}_{VM} = r_{VM} \Delta h'_{VM} = \frac{dM_{VM}}{dt} \Delta h'_{VM}$$

(12)

where $r_{VM}$ is the rate of volatile release (kg/s), $\Delta h'_{VM}$ is the heat of pyrolysis (kJ/kg), and $\Delta h'_{VM} = 420$ kJ/kg.\(^{16}\)

The heat generation from char’s combustion $\dot{Q}_C$ is given by eq 13.

$$\dot{Q}_C = r_C \Delta h_C = \frac{dM_C}{dt} \Delta h_C$$

(13)

where $r_C$ is the rate of consumption of char (kg/s), $\Delta h_C$ is the heat generation from char’s combustion, and $\Delta h_C = 21,000$ kJ/kg.\(^ {14}\)

4.3.3. Moisture Evaporation model. The change in the mass of moisture over time is similar to that of volatile matter. The rate of evaporation of moisture is determined using eq 14.

$$r_M = \frac{dM_M}{dt} = 37 \times 10^4 \exp\left(-\frac{4000}{T_P}\right) \times (M_{M,0} - M_{M,i})$$

(14)

where $M_{M,0}$ and $M_{M,i}$ are the initial mass of moisture and the total mass of moisture before time $i$ (kg), respectively.

4.3.4. Devolatilization Model. The chemical percolation devolatilization (CPD) model is a complex network model based on molecular structure. It has been reported to be useful in predicting the yield of volatile matter and product components during the rapid pyrolysis of coal. The model is more accurate than the simple kinetic devolatilization model.\(^ {26,27}\) In the present study, the devolatilization model of the single coal particle with moisture can be determined by the data iteration of the CPD model and the ignition model. The heating rate of the particle from the ignition model under different conditions was put into the CPD model, and the CPD simulation results were fitted as the devolatilization correlation until the iterations converged. The devolatilization correlation is given by eq 15. Therefore, the devolatilization correlation was related to the moisture content and particle size. The determination method and the accuracy of the devolatilization correlation are described in detail in the previous work.\(^ {14}\) The CPD model was also used to determine the total yield, volatile component yield, and heat of volatile chemical reaction ($h_{VM}$) under various conditions.\(^ {14}\) Some pyrolysis characteristic parameters from the CPD model are presented in Table 1.

| Table 1. Pyrolysis Characteristics of the Coal Particle (Particle Size of 125 µm) |
|-----------------|-----------------|-----------------|
| (moisture content (wt %)) | $h_{VM}$ (MJ/kg) | (VM yield (wt %)) | $R^2$ |
| 0               | 16.94           | 67.49           | 0.98631 |
| 5               | 16.80           | 67.06           | 0.99378 |
| 10              | 16.69           | 66.75           | 0.99436 |
| 20              | 15.96           | 64.54           | 0.98129 |

The correlation coefficient $R^2$ of the volatile released curves from the ignition model and the CPD model was above 0.98, indicating that the fitting correlation can reflect the simulation results of the CPD model in a satisfactory way. Meanwhile, the volatile yield of the sample was 67.49% (daf) from the CPD model, which was substantially higher than that of 41.7% (daf) from the proximate analysis conversion. Similar results also appeared in some previous studies.\(^ {28,29}\) Therefore, it can be said that the results of the CPD model can more accurately reflect the devolatilization process of coal.

$$r_{VM} = \frac{dM_{VM}}{dt} = \frac{P_{O_2,\infty}}{1 + \frac{1}{K_{n}}}$$

(16)

where $P_{O_2}$ is the specific surface area of the particle, $S_p = 18,000$ (m$^2$/kg), $K_{C}$ is the apparent reaction rate coefficient (kg/m$^2$/s/atm), $K_{n}$ is the mass transfer coefficient (kg/m$^2$/s/atm), and $P_{O_2,\infty}$ is the partial pressure of oxygen in the bulk gas (atm).

The apparent reaction rate coefficient is given by eq 17.

$$K_{C} = \eta \rho_p S_p A_0 \exp\left(\frac{-E}{R_s T_P}\right)$$

(17)

where $\eta$ is the effectiveness factor, $\gamma$ is the characteristic size of the particle (m), $\rho_p$ is the density of the particle (kg/m$^3$), $A_0$ is
the frequency factor, $A_v = 8.6 \times 10^7$ (kg/m²/s/atm), $E_v$ is the activation energy, $E_v = 150,000$ (kJ/mol), and $R_n$ is the gas constant with the value of 8.314 (J/K/mol).

The apparent reaction rate coefficient is given by eq 18.

$$ K_m = \frac{10M_{Sh}}{RT_p \rho \beta} \left( \frac{T}{1.5} \right) \frac{D_{ref}}{1.98 \times 10^{-1} \text{cm}^2/s} $$

(18)

where $M_{Sh}$ is the molecular weight of carbon, $R$ is the gas constant with the value of 82.06 (cm³·atm/mol·K), $Sh$ is the Sherwood number ($Sh = 2^{0.53}$), and $D_{ref}$ is the reference value of the diffusion coefficient.

4.3.6. Some Key Parameters. The diameter of the particle does not change during the release of moisture and volatile matter. However, the density of the particle changes during the process and is given by eq 19.

$$ \left( \frac{1}{6} \pi d_{ps} \right) \frac{d\rho_t}{dt} = \frac{dm_{vm}}{dt} - \frac{dm_{li}}{dt} $$

(19)

The diameter of the particle changes during the combustion of char, as shown in eq 20.

$$ \frac{d(d_p)}{dt} = -\frac{2}{\pi d_{ps}^2} \frac{\sigma_{\rho_t}}{\rho_t} d_{ps} $$

(20)

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