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# Thermal and kinetic analysis of pressurized oxy-fuel combustion of pulverized coal: An interpretation of combustion mechanism

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| <i>Keywords:</i><br>Pulverized coal<br>Pressurized oxy-fuel combustion<br>Thermogravimetric analysis<br>Combustion kinetic mechanism | Pressurized oxy-fuel combustion is one of the emerging clean technologies that can efficiently separate and recover CO <sub>2</sub> , and this combustion mechanism differs significantly from atmospheric air combustion. In this paper, the effects of reaction conditions such as total pressure, oxygen concentration and atmosphere gas composition on the combustion characteristics of Xinjiang Bostan coal were investigated using thermogravimetric methods. Furthermore, the thermodynamics parameters and the most probabilistic kinetic model for the pressurized oxy-fuel combustion process were explored. The results showed that the system pressure rising from 0.1 to 1 MPa could enhance the combustion process of coal; however, when the system pressure exceeds 0.5 MPa, the promoting effect is clearly weakened. The ignition mechanism transforms from heterogeneous to homogeneous when the oxygen concentration reaches 50% at 0.5 MPa. The mechanism functions of pressurized oxy-fuel combustion progressed. In addition, the rise of pressure and oxygen concentration correspond to the higher chemical reaction order of pulverized coal combustion and the pressure has less influence on the reaction mechanism than oxygen concentration. The results obtained may assist with the optimization of pressurized oxy-fuel combustion and guide its industrial applications. |

# 1. Introduction

Aimed at addressing climate change caused by CO<sub>2</sub> emissions, the consumption ratio of coal has been decreasing in China, while its total consumption is still on the rise. The power generation industry relies heavily on coal-fired power, which is responsible for more than 50% of the total coal consumption in primary energy production (Gopan et al., 2015; Lasek et al., 2013; Lv et al., 2021). Carbon dioxide capture and sequestration (CCS) technology is a promising strategy to alleviate the CO2 emissions from coal-fired power plants, as it allows for the effective control of emissions from concentrated locations (Chen et al., 2013; Engin et al., 2020). Oxy-fuel combustion (denoted as O<sub>2</sub>/CO<sub>2</sub> combustion) is widely regarded as a potential technology for CCS because of its relatively low cost, better accessibility for scale-up and fewer retrofitting requirements for existing stock units (Yang et al., 2021). In this process, air is replaced by a mixture of pure oxygen (>95%) from the air separation unit and recycled flue gas (mainly CO<sub>2</sub>) oxidizer for fuel combustion. The flue gas from oxy-fuel combustion primarily consists of CO2 and H<sub>2</sub>O. The liquid CO<sub>2</sub> is separated by a condensing unit, which only

requires dehydration to produce a high-purity (>90%  $CO_2$ ) gas stream. Meanwhile, other contaminants such as  $SO_2$  and  $NO_x$  are removed during the condensation process (Hamadeh et al., 2020; Geng et al., 2020; Liu, 2009; Bu et al., 2016). However, attendant challenges remain in applying the oxy-fuel combustion technique. The pressure difference between the oxy-fuel combustion process at atmospheric pressure and the previous air separation unit (ASU) and subsequent compression unit (CPU) at pressurized conditions leads to significant energy losses, resulting in the impairment of system economics due to increased  $CO_2$ recovery costs (Soundararajan and Gundersen, 2013).

Addressing the above issue, the concept of pressurized oxy-fuel combustion coal-fired power generation system was proposed by ThermoEnergy of the United States around 2000 (Chen et al., 2019). The whole process takes place at a higher pressure using pressurized oxy-fuel combustion technology, which could significantly diminish the power loss due to the huge pressure fluctuations. Furthermore, recent researches revealed that pressurized oxy-fuel combustion systems could bring numerous advantages: (1) Streamlined boiler equipment size and reduced infrastructure costs; (2) The latent heat of steam in the flue gas

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Received 20 December 2021; Received in revised form 19 August 2022; Accepted 9 September 2022 Available online 19 September 2022 1750-5836/© 2022 Elsevier Ltd. All rights reserved. can be recovered owing to the rising steam condensation temperature at high pressure; (3) The high pressure system can avoid air leakage and thus reduce CPU power consumption; (4) Enhanced burning rate of coal char and convective heat transfer rate. (5) Emission reduction of pollutants (Li et al., 2018). According to the techno-economic analyses of the pressurized oxy-fuel combustion system reported in the literature (Soundararajan and Gundersen, 2013; Hong et al., 2010; Zebian et al., 2012), the increase of net efficiency and the reduction of capital cost and electricity cost could be achieved in comparison with the atmospheric oxy-fuel combustion. Gopan et al. (2014) recently proposed a concept of a staged pressurized oxy-fuel combustion process with graded feedstock via Aspen Plus modeling. It was found that the net efficiency of the system was approximately 7% higher than that of "traditional" atmospheric oxy-fuel combustion applications (from 29.3% to 35.7-36.7%). Accordingly, Kim et al. (2021) presented an advanced supercritical pressurized oxy-combustion power plant with a wet flue gas recirculation system, the plant net efficiency improved by approximately 10% compared with that of a first-generation oxy-combustion power plant under atmospheric pressure. Thus far, the results of most studies on pressurized oxy-fuel combustion simulations have been consistent, i.e., the net efficiency of the plant reaches its maximum at an operating pressure of about 1.0 MPa (Shi et al., 2019; Yadav and Mondal, 2022).

Due to the operative difficulty of laboratory equipment for pressurized oxy-fuel combustion, most experimental studies were conducted at atmospheric conditions (Chen et al., 2013; Liu, 2009; Fan et al., 2008). Only a few studies were performed under a pressurized oxy-fuel atmosphere to illustrate the combustion mechanism. Wang et al. (2011) studied the effect of pressure on the combustion characteristics of bituminous coal and discovered that the ignition temperature might not increase linearly with rising pressure. However, pressure could switch the ignition mechanism of pulverized coal. Ying et al. (2016)) investigated the influence of coal rank, system pressure, oxygen concentration and coal char structure on the ignition characteristics of coal under O<sub>2</sub>/CO<sub>2</sub> atmosphere. The results suggested that the ignition temperature appeared to have an increasing/decreasing tendency when the pressure was enhanced, with the best combustion performance of coal at 1 MPa. Saastamoinen et al. (SJJA, 1996) found that elevating the total system pressure could increase the internal temperature of coal particles and significantly reduce the burnout time through a pressurized spouted fluidized bed. Yang et al. (2021) explored the movement and combustion characteristics of densified rice hull pellets in a fluidized bed combustor at elevated pressures, and discovered that the pressure and atmosphere change did not strongly affect the devolatilization process. However, the temperature of the volatile flame and char particles increased with pressure, whereas the burnout time of biomass particle reduced due to enhanced oxygen transport. MacNeil et al. (MSB, 1998) studied the effects of pressure (0.1-0.7 MPa), particle size and oxygen concentration on the combustion rate of semicoke, and they found that the combustion rate achieved the maximum at 0.5 MPa, whereas the influence of oxygen concentration on the combustion rate was more remarkable at high pressure.

The relevant works mainly focused on the ignition and combustion properties of pressurized conditions. In addition, the selection of pressure in each of these experiments spanned a relatively wide range, which could cause noticeable variation in the combustion characteristics. To date, few research has presented a deep understanding of how the pressure and atmosphere affect the coal combustion characteristics. Likewise, few studies included a systematic kinetic analysis of oxy-fuel combustion under pressurized conditions. Herein, a simultaneous experimental and kinetic study is performed to demonstrate the mechanism of pressurized oxy-fuel combustion of pulverized coal in a pressurized thermogravimetric analyzer. The effects of different reaction conditions (such as total system pressure, reaction atmosphere and oxygen concentration) on the coal combustion process are quantitatively explored. The most probabilistic mechanism function of oxy-fuel combustion process is then discussed, and the corresponding kinetic parameters are calculated. Our results may provide valuable data to promote the advancement of pressurized oxy-fuel combustion technology, and broaden its industrial applications.

# 2. Experimental section

#### 2.1. Preparation of coal sample

Bostan coal (from Xinjiang Province, China), a typical bituminous coal with low ash content, high volatility, and fixed carbon content was selected as the test sample in this work. Prior to the experiment, the raw coal was crushed, ground and sieved to a particle size in the range of 96–150  $\mu$ m, then dried at 108 °C for 5 h and sealed in a desiccator for storage before use.

The proximate and ultimate analyses of coal sample were performed according to Chinese national standards of GB/T212–2008. The properties are presented in Table 1.

# 2.2. Experimental apparatus and procedure

The pressurized oxy-fuel combustion experiments were implemented in a pressurized thermogravimetric analyzer (PTGA, Thermal Max500, Thermo Fisher Scientific Corporation, USA), which mainly consisted of a gas regulating unit, a weight monitoring unit and a pressure regulating unit. The overall schematic diagram of the instrument is shown in Fig. 1. The PTGA featured a theoretical maximum working temperature of 900 °C, maximum pressure of 7 MPa, balance sensitivity of 1  $\mu$ g, and weighing range of  $\pm 10$  g. The gas regulating unit was composed of three gas streams: pure N<sub>2</sub> was used as purge gas and furnace gas to protect the balance components and the furnace, and a mixture of O<sub>2</sub> and CO<sub>2</sub> was applied as the reaction gas to maintain a certain pressurized atmosphere during the experiment.

The experimental procedure was executed as follows: 20 mg coal sample was spread evenly in the center of the quartz crucible to form a very thin layer, thereby reducing the influence of the diffusion effect between particles. After flushing the furnace with pure N2 for about 20 min, the gas supply was switched to reaction gas (O<sub>2</sub>+CO<sub>2</sub>, the O<sub>2</sub> concentration varied from 21% to 50%) to reduce the gas flow disturbance for the hanging wire while maintaining a relatively high velocity to lower the diffusion effect. After comprehensive consideration and the results of the preliminary experiment, a flow rate of 0.4 L/min was selected. The reactor pressure was slowly elevated to the set value (0.1, 0.3, 0.5, 0.7, 1 MPa). The backpressure valve was adjusted to balance the inlet and outlet gas streams to ensure that the pressure of furnace remained stable during the combustion process. After the target pressure stabilized for 30 min, the furnace was heated up from room temperature to 900 °C at 25 °C/min, and the range of the linear temperature increase was 100~900 °C. During the course of heating up of the instrument, the sample weight and temperature were monitored online for analysis. It is worth noting that the increase of gas density under high pressure would cause the apparent weight gain of the quartz crucible, therefore, a blank experiment had to be carried out to eliminate the influence of buoyancy. Under each pressure condition, the operation with the blank sample was fully consistent with the experimental conditions, and the oxy-fuel combustion experiment of coal was subsequently carried out. Finally, using the same time span as the scale, the two sets of data were subtracted to obtain the experimental curve. Each experiment was implemented at least three times to ensure reproducibility and reliability.

# Table 1

Proximate and ultimate analyses of Bostan coal.

| Proximate analysis (wt%, ad) |      |       | Ultimate analysis (wt%, ad) |       |      |       |      |      |
|------------------------------|------|-------|-----------------------------|-------|------|-------|------|------|
| М                            | А    | V     | FC                          | С     | Н    | 0     | Ν    | S    |
| 1.36                         | 5.93 | 37.88 | 54.83                       | 70.88 | 4.60 | 15.37 | 1.37 | 0.49 |

ad = air dry basis; M = moisture; A = ash; V = volatile matters; FC = Fixed carbon.



Fig. 1. Schematic diagram of the PTGA system.

#### 2.3. Experimental data processing method

Ignition temperature and burnout temperature are important characteristic parameters reflecting the combustion characteristics of pulverized coal particles. In the practical industry, it is of great guiding significance to master these two key parameters for the ignition and stable combustion of coal fuel. There are many methods to define ignition temperature and burnout temperature using TG/DTG curves obtained from thermogravimetric experiments (Fan et al., 2008; Babinski et al., 2018), and the values of combustion characteristic temperatures obtained by different methods may vary to some extent. However, as long as a unified definition method is adopted in the research process, the experimental analysis results obtained will be comparable and credible. The tangent method of TG/DTG curve was used to define ignition temperature in this work. As shown in Fig. 2, draw a perpendicular line intersected TG curve at the maximum weight loss peak of DTG curve, and a tangent line of TG curve was made at this intersection



Fig. 2. Definitions of ignition temperature and burnout temperature.

point, which intersected with the initial weightlessness parallel line of TG curve. The temperature corresponding to this intersection point was defined as ignition temperature( $T_i$ ). The burnout temperature ( $T_b$ ) was defined as the temperature when the combustion conversion rate reaches 98% and remains stable in the whole process of weightlessness.

In order to evaluate the combustion performance under different atmospheres more comprehensively, the ignition index (C<sub>i</sub>, min<sup>3</sup>), burnout index(C<sub>b</sub>, %/min<sup>4</sup>), and comprehensive combustion characteristic index (S,%/ °C<sup>3</sup> × min<sup>2</sup>) were introduced to measure the combustion performance of pulverized coal, where the ignition index and burnout index represent the ability of coal to ignite and burn out during the combustion process. Higher C<sub>i</sub> and C<sub>b</sub> means higher ignition and burnout capabilities. The comprehensive combustion characteristic index S reflects the combustion performance of the sample, it contains the essential features combustion such as ignition temperature, burnout temperature and burning rates in various conditions. It functions as a general indication of combustion characteristics of the coal. Generally speaking, higher index S means better pulverized coal combustion qualities. These parameters were calculated using the following formula (Wang et al., 2011):

$$C_{\rm i} = \frac{(dw/dt)_{\rm max}}{t_i t_{\rm max}} \tag{1}$$

$$C_{b} = \frac{(dw/dt)_{max}}{\Delta t_{1/2} t_{max} t_{b}}$$
(2)

$$S = \frac{R}{E} \left[ \frac{d\left(\frac{dw}{dt}\right)}{dT} \right]_{T=T_i} \frac{(dw/dt)_{\max}}{(dw/dt)_{T=T_i}} \frac{(dw/dt)_{\max}}{T_b}$$

$$= \frac{(dw/dt)_{\max}(dw/dt)_{\max}}{T_i^2 T_b}$$
(3)

In the above equations,  $(dw/dt)_{max}$  represents the maximum reaction rate,%/min;  $(dw/dt)_{mean}$  is the average reaction rate,%/min;  $t_i$  refers to the ignition time, min;  $t_{max}$  is the time corresponding to the maximum reaction rate, min;  $t_b$  is the burnout time, min;  $\Delta t_{0.5}$  is the time of  $(dw/dt)/((dw/dt)_{max}=0.5, min.$ 

# 3. Results and discussion

#### 3.1. Effect of pressure on combustion characteristics of coal

The TG and DTG curves of Bostan coal under 30%O<sub>2</sub>/70%CO<sub>2</sub> atmosphere are shown in Fig. 3, as the pressure increases from 0.1 to 1 MPa. With the increase of environmental temperature, the reaction can be divided into three processes, dehydration, devolatilization and combustion. There are no sharp boundaries seen in the DTG curves, indicating that these processes overlap during the whole combustion. Devolatilization takes place earlier with the increase of pressure at the temperature range of 100~200 °C, resulting from the density changes of gas around the coal particles. The rising environmental pressure leads to the increase of reaction gas density. Meanwhile, the volume flow rate of the experiment remains constant, thus the actual mass flow rate of reaction gas keeps growing and, in the same capacity reactor, the pressurized reaction gas can accumulate more heat. Consequently, the higher heat capacity of the surrounding gas will obviously affect the initial heating process, resulting in the higher surface temperature of pulverized coal particles, which explains the advance of pyrolysis (SJJA, 1996). As environmental pressure increases, it becomes more challenging for internal volatile to escape from coal particles. This inhibition will result in higher concentration of volatiles in the stomata of solid particles and strengthening of the secondary reaction between volatiles, then cause an increase in gaseous products and correspondingly raise the internal pressure of sample particles. Forced convection would be formed when internal pressure exceeds external pressure, which allowing for faster and more efficient mass transport compared with normally diffusion in atmospheric environment, the volatile release rate also increases correspondingly. In the range of 300~500 °C, after being ignited, coal burns rapidly and its weight drops drastically, forming a peak corresponding to the maximum weight loss rate in the DTG curve, indicating that homogeneous ignition exists in this zone. Homogeneous ignition, heterogeneous ignition and combined ignition are three typical kinds of pulverized coal ignition mechanisms that can be distinguished by the relative magnitude of heating rate of the coal surface and release rate of volatiles (Essenhigh et al., 1989). The heating rate of particles in PTGA remains consistent (25 K/min), as a result, the rate of volatile release is the primary factor in determining the ignition pattern. Zhou et al. (2012) proposed a method to visually distinguish the ignition mechanism by the number of weightlessness peaks in DTG curves. Herein, only one peak can be observed (as displayed in Fig. 3 (b)), hence the variation of pressure from 0.1 to 1 MPa has no effect on the initially heterogeneous ignition mechanism of Bostan coal.

Generally speaking, the TG curves shift to a lower temperature zone with the elevated pressure and the correspondingly increased peak value of DTG curves, illustrating the significant enhancement of combustion rate. The boundary of volatiles' combustion and char combustion becomes gradually unclear, and the peaks of DTG are getting narrower and sharper. As known from the kinetics equations of the model-free method proposed by Liu (2009), the calculation of combustion rate can be described by Eq. (4), and the combustion rate of coal is positively correlated with the oxygen partial pressure. According to Dalton's law of partial pressure rises with increase of total pressure, which promotes the contact reaction between coal and oxygen, hence the reaction rate significantly increases.

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = k(T)f(\alpha)P_{\mathrm{O}_2}^m \tag{4}$$

where  $\alpha$  represents the conversion rate of coal,  $f(\alpha)$  is a structural factor, which is a function of  $\alpha$  and depends on the structural characteristics of coal particles,  $P_{O_2}^m$  represents the partial pressure of oxygen, and *m* is the reaction order. k(T) denotes the reaction rate parameter, which is determined by Arrhenius's equation as follows:

$$k(T) = A \exp\left(-\frac{E}{RT}\right)$$
(5)

where A denotes the pre-exponential factor, E denotes the activation energy of the whole reaction, and R is the gas constant.

It can be seen from Fig. 4 that the pressure increase can significantly reduce the ignition temperature and burnout temperature of coal. When the pressure rises from 0.1 MPa to 1 MPa, the ignition temperature of coal decreases by 66 °C, and the burnout temperature decreases by 116 °C. Under normal pressure, the volatiles released during the pyrolysis process hardly accumulate around the coal particles, but instead spread rapidly to the surface of coal. After the volatiles have escaped from the particles, the remaining porous char is more difficult to ignite. The uptrend pressure will affect the diffusion of reaction gas molecules, which in turn increases the release resistance of volatiles, resulting in more volatiles being confined inside the coal particles or accumulating on the surface of the particles, which could not be quickly released into the external environment. At this time, the pulverized coal is more likely to crack under the action of pressure difference between the internal and external particles, which makes the coal easier to ignite.

The enhancement of coal combustion becomes increasingly evident when the pressure rises from 0.1 MPa to 0.5 MPa. However, as the pressure further rises to 1 MPa, the effect of combustion promotion progressively weakens. The whole process of reaction gas can be regarded as steady-state diffusion, and according to Fick's first law, the oxygen diffusion flux (molar flow rate) at the interface of coal particles



Fig. 3. TG and DTG curves of coal combustion under different pressures.



Fig. 4. Combustion performance parameters of coal at different pressures.

can be defined by Eq. (6) (Babinski et al., 2018):

$$N_{\rm O_2} = \frac{D_{\rm O_2}}{h_{\rm D}} A_{\rm N} c({\rm O_2}) \tag{6}$$

where  $D_{O_2}$  represents the diffusion coefficient of oxygen,  $h_D$  represents the vertical distance between the top of crucible and the sample surface,  $A_N$  represents the horizontal cross-sectional area of the crucible, and  $c(O_2)$  denotes the concentration of oxygen.

In the thermogravimetric experiment, the flow rate of the reaction

gas is high enough, thus it can be assumed that the oxygen concentration does not change with time, and since all experiments are conducted using the same crucible, the value of  $h_D$  and  $A_N$  are consistent. Accordingly, we can infer that the diffusion flux of oxygen is only related to its diffusion coefficient. The diffusion coefficient of the binary mixture is generally calculated using the formula proposed by Fuller (Wang et al., 2011):



Fig. 5. TG and DTG curves of coal combustion under different atmospheres at 0.1 MPa and 0.5 MPa.

$$D_{12} = \frac{0.1013T^{1.75} \left(\frac{1}{M_1} + \frac{1}{M_2}\right)^{0.5}}{p \left[ \left(\sum v_1\right)^{1/3} + \left(\sum v_2\right)^{1/3} \right]^2}$$
(7)

where *p* represents the system pressure, *T* represents the system temperature,  $M_i$  represents the molar mass of gas molecules, and  $v_i$  represents the diffusion volume of gas molecules.

According to Eq. (7), when the oxygen concentration and heating rate are consistent, the rise of total pressure reduces the oxygen diffusion coefficient, delays the oxygen diffusion rate at the interface of coal particles, and weakens the pressure acceleration on coal combustion. Therefore, with the further increase of pressure, the growing trend of coal combustion rate slows down.

## 3.2. Effect of oxygen concentration on combustion characteristics of coal

The TG and DTG curves of coal under different atmospheres at 0.1 MPa and 0.5 MPa are shown in Fig. 5. If the system pressure and oxygen concentration remain unchanged, and the combustion atmosphere changes from  $O_2/N_2$  to  $O_2/CO_2$ , the TG curves shift slightly back to the higher temperature zone, and the DTG peaks decrease and shift backward, indicating the degradation of combustion performance, such as the increase in ignition temperature, the delay in burnout time, and decrease in combustion rate. Similar experimental phenomena have been observed by other researchers (Liu, 2009). The specific heat capacity of  $CO_2$  gas is higher than that of  $N_2$ ;  $CO_2$  absorbs more heat by raising the temperature to the same value, which reduces the surface

temperature of pulverized coal particles. Besides, according to Eq. (7), when the temperature, pressure and oxygen concentration are the same, the diffusion coefficient of  $O_2$  in  $CO_2$  is smaller than that in  $N_2$ , therefore, the oxygen supply rate reduces while the heat release rate of combustion decelerates. This makes it harder for coal to ignite and sustain combustion under an  $O_2/CO_2$  atmosphere than under an  $O_2/N_2$  atmosphere.

When the total pressure of the reaction system remains consistent, with the rise of oxygen concentration, the TG and DTG curves shift distinctly to the lower temperature zone and the DTG peaks increase drastically, indicating the significant improvement in the overall combustion performance with rising oxygen concentration. When the total pressure of the system remains unchanged, the increase of oxygen concentration indicates the rising partial pressure of oxygen according to the principle of reaction kinetic and Eq. (4), which could accelerate the rate of coal oxidation. In addition, according to Eq. (5) and Eq. (6), the diffusion coefficient of oxygen does not show considerable change when the total pressure of the system remains the same, however, the diffusion flux (molar flow rate) of oxygen is directly proportional to the oxygen concentration. Therefore, as the oxygen concentration increases, it promotes the diffusion of oxygen to the surface and inner layer of coal particles, and intensifies the contact between O2 and porous coal sample, thus greatly enhancing the combustion.

It can be seen from Fig. 6 that the ignition temperature of  $O_2/CO_2$ and  $O_2/N_2$  atmosphere are almost the same with fixed oxygen concentration, which reveals that in the lower temperature zone (100~300 °C), the difference between the effects of CO<sub>2</sub> and N<sub>2</sub> on the precipitation of volatiles is not obvious, but the burnout temperature under  $O_2/CO_2$ 



Fig. 6. Combustion performance parameters of coal under different atmospheres.

atmosphere is higher than that under O<sub>2</sub>/N<sub>2</sub> atmosphere, which is caused by the high specific heat capacity and low thermal diffusivity of CO<sub>2</sub>. Therefore, the comprehensive combustion characteristics of coal under O<sub>2</sub>/N<sub>2</sub> atmosphere are better than that under O<sub>2</sub>/CO<sub>2</sub> atmosphere (Engin et al., 2020; Chen et al., 2019; Yao et al., 2019). When the oxygen concentration increases, T<sub>i</sub> and T<sub>b</sub> show a downward trend, and the comprehensive combustion characteristics of coal have been further strengthened. It is worth noting that at atmospheric pressure, the growth tendency of comprehensive combustion characteristics gradually slows down with the rise of oxygen concentration, however, at the pressure of 0.5 MPa, the increasing tendency becomes stronger, indicating that pressurized oxy-fuel combustion has a significant effect on improving the ignition and combustion characteristics of coal. When the oxygen concentration reaches 50% at 0.5 MPa, the simultaneous increase in pressure and oxygen concentration significantly accelerates the pyrolysis process of coal, thus volatile release rate exceeds the heating rate of coal particle, consequently the ignition mechanism transforms from heterogeneous to homogeneous. Under normal pressure, the improvement of combustion performance by elevating the oxygen concentration is very limited, however, under low pressure (such as 0.5 MPa, which is easy to achieve in the industry), increasing oxygen concentration can significantly improve the coal combustion performance. In summary, pressurized oxy-fuel combustion is an operation method that is expected to remarkably improve fuel combustion performance. Some fuels with poor comprehensive combustion characteristics, such as biochar, petroleum coke, garbage, etc., may be able to utilize this new combustion technology.

#### 4. Kinetic analysis of oxy-fuel combustion reaction

#### 4.1. Reaction kinetic analysis method

Coal combustion, which involves a series of chemical and physical processes, is fairly complicated. The non-isothermal method is mainly carried out to analyze the dynamics of this process, which can be further divided into the integral method and the differential method. However, the differential method usually produces a large error, therefore, based on previous research experience and comprehensive consideration, the Coats-Redfern integral method is employed in this study to explore the kinetic mechanism of pressurized combustion reaction.

The Coats-Redfern integral method belongs to single scan rate methods with a fixed program heating rate. In the pressurized oxy-fuel combustion experiment, the time required for the pressurization process and the complete replacement of the reaction atmosphere under high pressure lasts very long, so the chosen method can improve the efficiency and obtain more reliable dynamic parameters. According to Eq. (4) and Arrhenius' law, the reaction rate of pulverized coal combustion can be defined as follows:

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = A \exp\left(-\frac{E}{RT}\right) f(\alpha) P_{\mathrm{O}_2}^m \tag{8}$$

$$\alpha = \frac{m_0 - m}{m_0 - m_\infty} \tag{9}$$

$$\beta = \frac{dT}{dt} \tag{10}$$

Using Eq. (10), Eq. (8) can be transformed as follows:

$$\frac{\mathrm{d}\alpha}{f(\alpha)} = \frac{A}{\beta} \exp\left(-\frac{E}{RT}\right) P_{O_2}^m dT \tag{11}$$

For this study, the reaction gas flow velocity is high enough and oxygen is supplied at a much faster rate than oxygen consumption, thus the oxygen partial pressure is considered unchanged during the whole combustion process of coal particles. The parameter *m* is taken as unity. For the convenience of calculation,  $A*P_{02}^{m}$  is defined as a new pre-

exponential factor including the influence of partial pressure for oxygen, represented by  $A_0$ . Applying the Coats-Redfern integration of Eq. (11) yields the following formula:

$$G(\alpha) = \int_{0}^{\alpha} \frac{d\alpha}{f(\alpha)} = \frac{A_0}{\beta} \int_{0}^{T} \exp\left(\frac{E}{RT}\right) dT = \frac{A_0}{\beta} \frac{RT^2}{E} \left(1 - \frac{2RT}{E}\right) \exp\left(-\frac{E}{RT}\right)$$
(12)

For the coal combustion process,  $\frac{2RT}{E} \ll 1$  and  $1 - \frac{2RT}{E} \approx 1$ , thus, after mathematical transformation, Eq. (11) becomes:

$$\ln\left[\frac{G(\alpha)}{T^2}\right] = \ln\left(\frac{A_0R}{\beta E}\right) - \frac{E}{RT}$$
(13)

Let the left side of Eq. (13) be *y*, and 1/T be *x*. A line can be obtained from the plot of *y* and *x*. Here, the *E* and  $A_0$  values can be extracted from the slope and intercept of the linear fitting, respectively. A summary of the most common and validated combustion mechanisms is shown in Table 2:

#### 4.2. Method of inferring the most probabilistic kinetic model

The present study is based on the integral method to obtain the kinetic parameters of the oxy-fuel combustion of coal. Notably, the temperature integral does not have the exact analytical solution in the process of integral solving, and it can only be calculated using approximate solutions. In addition, the selection of different reaction mechanism functions f ( $\alpha$ ) also has a certain influence on the value of activation energy, therefore, choosing the most probabilistic kinetic model is of great help to describe the reaction process more aptly. The Malek method is a relatively complete and accurate thermal dynamic analysis method, which is based on the shape and eigenvalue of the definition function converted from experimental data to infer the form of the mechanism function.

The function  $y(\alpha)$  in Malek's method is defined as follows:

| Table 2 |  |
|---------|--|
|---------|--|

| Summary of the most common and | validated | combustion | mechanisms |
|--------------------------------|-----------|------------|------------|
|--------------------------------|-----------|------------|------------|

| Species                                 | Mechanism                           | Symbol | f(α)  | G(α)                               |
|---|-------------------------------------|--------|---|------------------------------------|
| Reaction order<br>model                 | First-order reaction                | F1     | (1-α)   | -ln(1-α)                           |
|   | Second-order<br>reaction            | F2     | (1-α)   | $(1-\alpha)^{-1}-1$                |
|   | Third-order<br>reaction             | F3     | (1-α)   | $0.5[(1-\alpha)^{-2}-1]$           |
| Power function<br>model                 | Power law 1                         | M1     | 1   | α                                  |
|   | Power law 2                         | M2     | $2\alpha^{1/2}$   | $\alpha^{1/2}$                     |
|   | Power law 3                         | M3     | $3\alpha^{2/3}$   | $\alpha^{1/3}$                     |
| Nucleation and<br>growth model<br>(JMA) | Avrami-Erofeev                      | A2     | $2(1-\alpha)[-ln (1-\alpha)]^{1/2}$                               | $[-\ln(1-\alpha)]^{1/2}$           |
|   | Avrami-Erofeev                      | A3     | $3(1-\alpha)[-ln (1-\alpha)]^{2/3}$                               | $[-\ln(1-\alpha)]^{1/3}$           |
|   | Avrami-Erofeev                      | A4     | $4(1-\alpha)[-ln (1-\alpha)]^{3/4}$                               | $[-\ln(1-\alpha)]^{1/4}$           |
| Phase interface<br>reaction             | Shrinking cylinder<br>(area)        | R2     | $2(1-\alpha)^{1/2}$   | $1 - (1 - \alpha)^{1/2}$           |
|   | Shrinking spherical (volume)        | R3     | $3(1-\alpha)^{2/3}$   | $1 - (1 - \alpha)^{1/3}$           |
| Diffusion model                         | One-dimensional diffusion           | D1     | $1/2\alpha$   | α                                  |
|   | Two-dimensional<br>diffusion        | D2     | $[1-\ln(1-\alpha)]^{-1}$  | $[(1-\alpha)\ln(1-\alpha)]+\alpha$ |
|   | Three-dimensional diffusion(Jander) | D3     | $3/2 (1-\alpha)^{2/3}$<br>$^{3} [1-(1-\alpha)^{1/3}]$             | $[1-(1-\alpha)^{1/3}]^2$           |
|   | Three-dimensional diffusion eqn.3D  | D4     | $6 (1-\alpha)^{2/3}$<br>[1-(1- $\alpha$ ) <sup>1/</sup><br>31 1/2 | $[1-(1-\alpha)^{1/3}]^{1/2}$       |

$$y(\alpha) = \frac{f(\alpha) \cdot G(\alpha)}{f(0.5) \cdot G(0.5)}$$
(14)

among the above parameters,  $f(\alpha)$  represents the reaction mechanism function, and  $G(\alpha)$  is its integral form. The standard curve  $y(\alpha)$ - $\alpha$  of any reaction mechanism function can be obtained from Eq. (14) in conjunction with Table 2, and the experimental curve can be obtained by substituting the experimental data into Eq. (15):

$$y(\alpha) = \left(\frac{T}{T_{0.5}}\right)^2 \frac{\left(\frac{d\alpha}{dt}\right)}{\left(\frac{d\alpha}{dt}\right)_{0.5}}$$
(15)

where  $T_{0.5}$  and  $d\alpha / dt$  are respectively the temperature and reaction rate when  $\alpha$ =0.5. When the experimental curve overlaps with the standard curve, the *f* ( $\alpha$ ) corresponding to the standard curve can be regarded as the most probable kinetic mechanism model.

#### 4.3. Kinetic study of pressurized oxy-fuel pulverized coal combustion

Many scholars have studied the kinetics of atmospheric oxy-fuel combustion, and they consistently found that the chemical reaction order model could well fit the entire combustion process (Wang et al., 2021). In this study, the first order chemical reaction model is tentatively used for kinetic calculation. When the mechanism model does not conform to the experimental data, the most probable model is inferred by the Malek method.

The fitted straight lines of the activation energy measured by Coats-Redfern integral method under different pressures (0.1/0.3/0.5/0.7/1 MPa) in 30%O<sub>2</sub>/70% CO<sub>2</sub> atmosphere are shown in Fig. 7. The calculated results are listed in Table 3. Overall, the correlations of the fitted curves are all greater than 0.99, indicating that the hypothesis of the chemical first order reaction kinetic model is reasonable for pressurized oxy-fuel pulverized coal combustion.

According to the widely accepted theory of reaction kinetics, the value of the activation energy reveals the difficulty of the reaction. Based on the experimental results, higher pressure can promote the oxy-fuel combustion reaction, therefore, the activation energy should be correspondingly lower. However, it can be seen from Table 3 that apparent activation energy increases slightly with the pressure rising from 0.1 to 1 MPa. The combustion of pulverized coal is regarded as its oxidation in a stepwise process. As the temperature rises, the exposed and active components in coal react firstly with oxygen, which reactions require less energy, reducing the apparent activation energy. With the

Table 3

| Kinetic parameters of coa | l combustion under | different pressures |
|---------------------------|--------------------|---------------------|
|---------------------------|--------------------|---------------------|

| Pressure<br>p/MPa | Temperature<br>t∕ °C | Activation<br>energy/Ea<br>(kJ*mol <sup>-1</sup> ) | Pre-<br>exponential<br>factor A/s <sup>-1</sup> | Correlation<br>index R <sup>2</sup> |
|-------------------|----------------------|--|---|-------------------------------------|
| 0.1               | 386–536              | 83.64  | 3.61E+05  | 0.9966                              |
| 0.3               | 355-476              | 90.82  | 4.17E+06  | 0.9986                              |
| 0.5               | 330-443              | 92.38  | 1.22E + 07                                      | 0.9972                              |
| 0.7               | 320-429              | 94.87  | 2.86E+07  | 0.9973                              |
| 1.0               | 320-420              | 96.73  | 5.45E+07  | 0.9975                              |

further increase of temperature, the more stable structure of coal and its components gradually expose and ulteriorly react with oxygen; such oxidation reactions increase energy and may lead to higher apparent activation energy. As shown in Fig. 3, higher pressure causes the entire combustion reaction process to move towards the lower temperature zone, with the above-mentioned more difficult oxidation reactions occurring in this temperature zone, resulting in the enhancement of the apparent activation energy of the overall combustion process (Chansa et al., 2020). Moreover, Chen et al. (2013) considered that the activation energy of the sample is affected by the activation molecule concentration, diffusion restriction and organic impurities during combustion. Higher pressure will inhibit the precipitation of volatiles at the beginning of combustion.

Fig. 8 provides the Coats-Redfern kinetic analysis of the pulverized coal oxy-fuel combustion behaviors at 0.1 MPa under different atmospheres, and the corresponding kinetic parameters are listed in Table 4. Clearly, the correlations of the fitted curves are all greater than 0.99 under different atmospheres and oxygen concentrations, revealing that the assumption of the chemical first-order reaction kinetic model is reasonable. Compared with the increasing pressure, the elevating oxygen concentration makes the slope of kinetic fitting curve change more distinctly, suggesting that the sensitivity of pulverized coal oxy-fuel combustion reaction to oxygen concentration is higher than that to pressure. As can be seen from Table 4, the higher the O<sub>2</sub> concentration, the greater the apparent activation energy of the pulverized coal. In fact, with the increase of oxygen concentration, the total reaction temperature region narrows and a series of violent oxidation reactions occurring in lower temperature zone, which corresponds to a higher energy barrier, therefore leading to the rise of apparent activation energy. In addition, higher oxygen concentration causes the coal particles to burn rapidly and generate ash that effectively coats on the surface of coal char, thus hindering the internal burning of coal in lower temperature



Fig. 7. Kinetic fitting curve of pulverized coal under different pressures-



Fig. 8. Kinetic fitting curves of in different atmospheres at 0.1 MPa.

Table 4Kinetic parameters of coal under different atmospheres at 0.1 MPa.

| Atmosphere                                    | Temperature<br>t∕ °C | Activation<br>energy/Ea<br>(kJ*mol <sup>-1</sup> ) | Pre-<br>exponential<br>factor /s <sup>-1</sup> | Correlation<br>index R <sup>2</sup> |
|---|----------------------|--|--|-------------------------------------|
| 21%<br>O <sub>2</sub> +79%<br>N <sub>2</sub>  | 403–582              | 72.83  | 2.78E+04                                       | 0.9953                              |
| 21%<br>O <sub>2</sub> +79%<br>CO <sub>2</sub> | 402–614              | 62.06  | 3.45E+03                                       | 0.9943                              |
| 30%<br>O <sub>2</sub> +70%<br>CO <sub>2</sub> | 386–536              | 83.64  | 3.61E+05                                       | 0.9967                              |
| 40%<br>O <sub>2</sub> +60%<br>CO <sub>2</sub> | 382–501              | 98.66  | 9.07E+06                                       | 0.9989                              |
| 50%<br>O <sub>2</sub> +50%<br>CO <sub>2</sub> | 372–488              | 102.17   | 2.54E+07                                       | 0.9940                              |

zone. In previous studies, many people have also found that the apparent activation energy increases with the increase of oxygen concentration. Chansa et al. (2020) also used the Coats-Redfern method to calculate the kinetic parameters of coal oxy-combustion, he thought at higher oxygen percentage, its partial pressure would increase and made oxygen diffuse more to the fuel surface thereby increased the number of fuel's molecular structures reacting with oxygen. This phenomenon would lead to increasing temperature and thereby rinsed the apparent activation energy. Yi et al. (2014) proposed that the high reactivity of coal in oxygen-rich atmosphere leads to high apparent activation energy. Chen et al. (2013) adopted KAS and FWO methods at multiple heating rates to calculate reaction kinetic parameters, and also found that the average apparent activation energy increased with the increase of oxygen concentration, he thought as oxygen concentration raised, heat release from semi-coke oxidization increased and thus the surface temperature of semicoke elevated. Also, the semi-coke structure expanded the grain size and increased ash content corresponding to an increase in final temperature. Therefore, the activation energy increased with higher oxygen concentration. Yao et al. (2019) calculated the reaction kinetic parameters of semi-coke oxygen-rich combustion using the Starink method without assuming the reaction mechanism function. He discovered that the apparent activation energy decreased as the conversion rate increased during the combustion reaction. The average apparent activation energy of the whole combustion process increased as the oxygen concentration raised. He considered that the activation energy of the sample was affected by the decrease of activation molecule concentration, diffusion restriction and organic impurities during combustion.

The apparent activation energy under  $O_2/CO_2$  decreases by 10.77 kJ/mol than that under  $O_2/N_2$  with the same  $O_2$  concentration, which is consistent with the literature. The reason is that under  $O_2/CO_2$  atmosphere, the overall combustion characteristics of coal are less favorable than those under  $O_2/N_2$  atmosphere, the total reaction temperature region broadens and moves towards the high temperature zone. Besides, the specific heat capacity of  $CO_2$  gas is higher than that of  $N_2$ , it absorbs more heat by increasing the temperature to the same value. This reduces the surface temperature of coal particles and lowers the apparent activation energy.

Fig. 9 shows the results of Coats-Redfern kinetic analysis of pulverized coal oxy-fuel combustion behaviors at 0.5 MPa under different atmospheres, and the corresponding kinetic parameters are listed in Table 5. It is obvious that the correlations of the fitted curves are greater than 0.99 when the oxygen concentration is below 40%, As the oxygen concentration further rises to 50%, the combustion is clearly divided into two stages. The first-order kinetics model of chemical reaction is used for segmental fitting, however, according to the fitting results, the correlation between the model and the experimental curve weakens, indicating that, in the pressurized oxy-fuel of high oxygen concentration, the combustion mechanism of pulverized coal has changed. The possible reason is that the pulverized coal heats up in a high oxygen concentration under a certain pressure, the volatile drives off and quickly reacts with oxygen and then ignites violently. However, the temperature at this time is not high enough to ignite the residual char, therefore, the residual char oxidizes slowly instead of burning intensely.

As can be seen from Table 5, the increase of oxygen concentration under pressure will gradually slow down the rising trend of activation energy when the oxygen concentration is lower than 40%. However, when it reaches 50%, the average activation energy of the entire combustion reaction section suddenly rises to 144.07 kJ/mol, and the reaction temperature range shortens rapidly. Combined with the abovementioned facts, due to the high oxygen concentration and pressurized condition, the collision between molecules is highly intense, the ignition temperature of pulverized coal decreases sharply, and the severe combustion reaction takes place at a lower temperature zone. However, since the temperature of pulverized coal at this time is too



Fig. 9. Kinetic fitting curves of pulverized coal combustion under different atmospheres at 0.5 MPa.

 Table 5

 Kinetic parameters of coal under different atmospheres at 0.5 MPa.

| Atmosphere                                    | Temperature<br>t∕ °C | Activation<br>energy/Ea<br>(kJ*mol <sup>-1</sup> ) | Pre-<br>exponential<br>factor A/s <sup>-1</sup> | correlation<br>index R <sup>2</sup> |
|---|----------------------|--|---|-------------------------------------|
| 21%<br>O <sub>2</sub> +79%<br>N <sub>2</sub>  | 349–483              | 82.72  | 9.13E+05  | 0.99902                             |
| 21%<br>O <sub>2</sub> +79%<br>CO <sub>2</sub> | 349–500              | 75.53  | 1.80E+05  | 0.99651                             |
| 30%<br>O <sub>2</sub> +70%<br>CO <sub>2</sub> | 330–443              | 92.38  | 1.22E+07  | 0.99724                             |
| 40%<br>O <sub>2</sub> +60%<br>CO <sub>2</sub> | 302–404              | 96.30  | 7.68E+07  | 0.99095                             |
| 50%<br>O <sub>2</sub> +50%<br>CO <sub>2</sub> | 295–331<br>331–390   | 215.51<br>5.70                                     | 3.31885E+19<br>0.436022866                      | 0.91846<br>0.97781                  |

low, the apparent activation energy required for the reaction is correspondingly higher. Moreover, according to the principle of reaction kinetics, for the same gas-solid reaction, the lower the temperature, the greater the apparent activation energy required for the reaction. In summary, the trend of apparent activation energy with different pressures and oxygen concentrations is shown in Fig. 10.

#### 4.4. Kinetic model of coal pressurized oxy-fuel combustion process

In fact, the coal combustion process is a highly complex gas-solid reaction composed of three main subprocesses: outer gas diffusion, inner gas diffusion, and interface chemical reaction. These coexist and play dominant roles in different stages of the reaction. Accordingly, the change of apparent activation energy is partly caused by the change of reaction mechanism (Yao et al., 2019). Based on the previous calculation results, the first-order kinetics model of chemical reaction (F1), which is suitable for atmospheric oxy-fuel combustion as confirmed by most researchers, but its fitness decreases for high oxygen concentration pressurized oxy-fuel combustion. Therefore, it is necessary to infer the most probabilistic kinetic model of pulverized coal under different combustion states, which is helpful to establish a more accurate kinetic model of pressurized oxy-fuel combustion.

The process of inferring and confirming the most probable



Fig. 10. Distribution of activation energy in coal pressurized oxyfuel combustion.

mechanism model of the reaction is shown in Fig. 11. The standard curve  $y(\alpha)$ - $\alpha$  of every possible reaction mechanism function model can be obtained from Eq. (14) in conjunction with Table 2, and the experimental curve can be obtained by substituting the experimental data into Eq. (15).

When comparing the coincidence degree of the experimental curve and the standard curve, it can be found that most of the experimental curves cannot be completely matched with a certain standard curve. As the temperature rises and the combustion progresses, the reaction mechanism also changes accordingly. The most probabilistic kinetic model of coal oxy-fuel combustion is more likely to change when the conversion rate is <0.2 or >0.55. The multi-step reaction of coal pressurized oxy-fuel combustion gradually shifts from homogeneous reaction to heterogeneous reaction. The weakly connected hydrocarbon molecules in coal have been consumed in the previous step, promoting



Fig. 11. Curves of the most probabilistic mechanism function of the coal samples under (a) different pressures, (b) different atmospheres at 0.1 MPa, and (c) different atmospheres at 0.5 MPa.

the further pyrolysis and combustion of strongly linked hydrocarbon molecules and residual coal char, which eventually leads to the char burning out.

For oxy-fuel combustion under atmospheric pressure condition, especially in low oxygen concentration under O<sub>2</sub>/CO<sub>2</sub> atmosphere and  $O_2/N_2$  atmosphere, we find that the shape of the  $y(\alpha)$ - $\alpha$  curve presents a more noticeable change, suggesting that oxygen concentration may influence the mechanism function. The combustion reaction is evidently divided into two stages. The first stage is dominated by chemical kinetic reaction. Meanwhile, due to the lower temperature and reduced accumulation of ash, the reaction gas can easily pass through the solid product layer into the inside of the coal particle and react with it. The applicable mechanism functions at this stage are chemical reaction order model F1 with the integral function of the kinetic model  $[-\ln(1-\alpha)]$ , or phase interface reaction model R2 with the integral function of the kinetic model  $[1-(1-\alpha)^{1/2}]$ . The second stage of the combustion reaction is dominated by the diffusion effect. At this time, the reaction temperature is high and the ash has gradually accumulated on the surface of the coal particles, thus the diffusion of reaction gas and product gas is hindered. The mechanism function applied to this stage is a three-dimensional diffusion control model D4, with the integral function of the kinetic model  $[1-(1-\alpha)1/3]^{1/2}$ . When the oxygen concentration is higher than 30%, the most probabilistic mechanism function of the coal is relatively stably the chemical reaction order model F1, indicating that the excessively high oxygen concentration has less influence on the mechanism function, which is consistent with the results of previous studies (Yao

# et al., 2019; Wang et al., 2021).

Under the pressurized oxy-fuel combustion condition, when the oxygen concentration remains constant, with the increase of pressure, the overall combustion process is still mainly controlled by the chemical reaction. In addition, the corresponding reaction mechanism has the tendency to switch from the first-order reaction to the second-order reaction. Under the condition of pressurization, the increase of oxygen concentration makes the mechanism function change gradually from the first-order reaction to the third-reaction. Indicating that the rise of pressure and oxygen concentration both correspond to the higher chemical reaction order of pulverized coal combustion and the pressure has less influence on the reaction mechanism than oxygen concentration.

#### 5. Conclusions

In this paper, the thermal and kinetic behavior of the coal pressurized oxy-fuel combustion process were studied by thermogravimetric analysis, and the effects of pressure, atmosphere and oxygen concentration on the ignition and comprehensive combustion characteristics of pulverized coal were investigated. The mechanism function model suitable for pressurized oxy-fuel combustion was determined from the perspective of reaction kinetics. The following main conclusions can be drawn:

- (1) The system pressure rising from 0.1 to 1 MPa could enhance the combustion process of coal; however, when the system pressure exceeds 0.5 MPa, the promoting effect is clearly weakened, and combustion could also be improved significantly when the oxygen concentration reaches 50%. In terms of the economic cost of pressurized oxy-fuel combustion power plants, Perhaps the operation parameters of 0.5 MPa and 50%  $O_2$  can be regarded in the succeeding industrial operation.
- (2) Compared with atmospheric oxy-fuel combustion, the increase of oxygen concentration during pressurized oxy-fuel combustion can accelerate coal ignition and dramatically change the comprehensive combustion characteristics. The transition between the volatilization combustion stage and the carbon combustion stage under an atmospheric low oxygen concentration environment is relatively more vague, and the ignition mechanism is heterogeneous ignition. With the rise of pressure and oxygen concentration, the transition becomes more explicit and the ignition mechanism transforms from heterogeneous to homogeneous when the oxygen concentration reaches 50%.
- (3) The apparent activation energy of the combustion reaction increases with rising pressure and oxygen concentration. The intense combustion reaction has taken place at the lower temperature zone, which correspondingly requires larger apparent activation energy. Besides, elevated pressure and oxygen concentration cause the surface of coal particles to burn rapidly and generate ash that effectively coats on the surface of coal char, thus hindering the internal burning of coal.
- (4) The mechanism functions of pressurized oxy-fuel combustion reaction varied as the reaction progressed. The rise of pressure and oxygen concentration both correspond to the higher chemical reaction order of pulverized coal combustion and the pressure has less influence on the reaction mechanism than oxygen concentration.

# CRediT authorship contribution statement

Jiqing Yan: Conceptualization, Methodology, Validation, Investigation, Data curation, Writing – original draft, Writing – review & editing, Visualization. Mengxiang Fang: Resources, Writing – review & editing, Supervision, Project administration, Funding acquisition. Tong Lv: Investigation, Data curation. Yao Zhu: Investigation, Data curation. Jianmeng Cen: Resources, Funding acquisition. Yiming Yu: Investigation. Zhixiang Xia: Investigation. Zhongyang Luo: Resources, Project administration, Funding acquisition.

## **Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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