



Gasification and combustion kinetics of a high-ash-fusion-temperature coal using thermogravimetric analysis

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Abstract

The gasification/combustion kinetics of a typical Chinese high-ash-fusion-temperature (AFT) coal char, Huainan (HN) coal char, are analyzed using a thermogravimetric analyzer in this paper. The carbon conversion rate and the gasification/combustion reaction rate characteristics of HN coal char are studied. The initial gasification/combustion reaction rates are also analyzed in this paper. Results show that at 1300 °C, the gasification and combustion processes are changed from the chemical reaction control zone to the pore diffusion control zone. Thus, 1300 °C is recommended as the gasification temperature of the non-slagging EFGs system using high-AFT HN coal. Based on the isothermal method, a complementary method of iso-conversional and model based is used to analyze the gasification and combustion kinetics of HN coal char. The gasification/combustion reaction order m and activation energy E of HN coal char are obtained by iso-conversional method. The kinetic model equation $f(\alpha)$ is obtained based on a modified master plot method. The kinetic exponent n and the pre-exponential factor k_0 are obtained by model-based method. The results of this work provide the useful data for designing the non-slagging EFGs using high-AFT coals.

Keywords High-ash-fusion-temperature coal · Kinetics · Complementary method · Gasification · Combustion

Introduction

Entrained flow gasification technology has shown the great benefits (feasible, highly efficient, economical and environmentally friendly) on the large-scale conversion of coal and biomass into syngas for the synthesis of chemicals or energy utilization [1]. In entrained flow gasifiers (EFGs), pulverized coal particles were fed into the gasifier in dry (using N₂ or CO₂ as a transport gas) or wet (carried in a slurry water) manner and reacted with steam and oxygen or air in a suspension mode.

Slagging operations are all used in the existing EFGs, and up to 1500–1600 °C of the gasifier temperature is usually adopted in order to protect the gasifier refractory wall and ensure the high cold gas efficiency [2]. Meanwhile, the operation temperature of EFGs should be above the ash fusion temperature (AFT) of coal forming the liquid slag and promising the stable and steady drain of ash [3]. As a result, coals with the AFT below 1500–1600 °C are suitable for use in EFGs, for example, both GE/Texaco and Shell gasifiers recommend using the coal with the AFT of 1400 °C [4]. China is a major coal-producing country; however, the low-AFT coals only account for 40% of the total coal production [5], which could not satisfy the great consumption from coal chemical industries, including coal gasification.

Non-slagging (dry-bottom) EFGs are proposed in this work for gasification of high-AFT coals instead of paying the high price for slagging. In the non-slagging mode, which has been well performed in both 0.5 kg h⁻¹ bench-scale and 20 kg h⁻¹ pilot-scale gasifiers, the operation temperature is lower than the AFT of coal. Moreover, Wu et al. [6], Liu et al. [7, 8] and Kajitani et al. [9, 10] examined the gasification performance of the high-AFT and low-AFT coals.

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Results show that increasing gasification temperature above the AFT was not much help to improve the char gasification rate for all types of examined coal. Therefore, non-slagging gasification of high-AFT coals is an achievable goal in respect of the char gasification performance at the temperature below that of AFT.

The gasification performance of the high-AFT coals under such temperature is the key parameter in determining the feasibility of non-slagging EFGs. Wu et al. [6] analyzed the gasification reactivity of three high-AFT coals and one low-AFT coal via the isothermal thermogravimetric (TGA) at the temperature of 1100–1400 °C in CO₂ and H₂O atmospheres. The transition of gasification reaction from chemical reaction control (Regime I) to pore diffusion control (Regime II) occurred below the AFT of individual coal. And the temperature of the transition for the high-AFT coal was higher than that of the low-AFT coal.

In the aspect of kinetics, two main mathematic methods are the isothermal and non-isothermal methods [11]. Considering the heating rate of TGA is not exactly the same as that of the gasifier, the isothermal method is used in this work. Moreover, the mathematic methods can also be classified into iso-conversional (model-free) and model-based (model-fitting) methods [12]. Each method has advantages and disadvantages. Iso-conversional methods give an estimate of activation energy without model-based assumption [13–15], but it can only determine the activation energy. On the contrary, a reaction model must be postulated first in model-based methods [16, 17]; however, it can produce misleading results. Khawam and Flanagan [18] recommended a complementary method of iso-conversional and model based in the analysis of kinetics. This method was used in our previous work, and it showed high accuracy in kinetic calculation.

In the present work, the non-slagging gasification kinetic of a typical Chinese high-AFT coal char, Huainan coal char, is analyzed using a thermogravimetric analyzer. Moreover, the combustion reaction also exists in the gasification process. Thus, the combustion kinetic of Huainan coal char is also analyzed in this paper. The isothermal method was used to analyze the gasification and combustion kinetics of

Huainan coal char. In addition, a complementary method of iso-conversional and model based was also used to determine the pre-exponential factors and the reaction models. The results of this work provide the useful data for designing the non-slagging EFGs using high-AFT coals.

Experimental

Materials

Huainan (HN) coal from Huainan coal-mining area in China was selected in this work to be representative of AFT coals. Table 1 gives the characterization of HN coal, in which the proximate, ultimate analysis of the tested coal was conducted according to the Chinese standards GB/T212-2008, GB/T214-2007, GB/T476-2008, GB/T19227-2008, GB/T213-2008 and GB/T 219-2008. As can be seen, the fusion temperature of HN coal is very high, above 1500 °C.

Experimental method

HN coal char used in this work was obtained by heating HN coal from ambient temperature to 850 °C at a heating rate of 10 °C min⁻¹ under nitrogen atmosphere and then remained at 850 °C for 30 min. A high-temperature thermogravimetric analyzer (PE-STA-80000) was used in this work to study the gasification and combustion kinetic analysis of HN coal char. A sample of about 20 mg was put into an Al₂O₃ container without lid, placed in the thermal analyzer. The gasification of HN coal char was performed twice before experiments, and the results confirm the good repeatability of the TG system.

The temperature range for both gasification and combustion was set to be from 1100 to 1400 °C at a heating rate of 25 °C min⁻¹. Carbon dioxide and nitrogen were used as inert gases of the gasification process. Oxygen and nitrogen were used in the combustion process. The CO₂ partial pressure for gasification condition was set as 45, 55, 65 and 75%. The O₂ partial pressure for gasification condition was set as 5, 10, 15 and 21%. The detailed experimental conditions are listed in

Table 1 Proximate and ultimate analysis of HN coal

Proximate analysis/%				Ultimate analysis/%					HV/MJ kg ⁻¹	
M _{ad}	A _{ad}	V _{ad}	FC _{ad}	C _{ad}	H _{ad}	O _{ad}	N _{ad}	S _{ad}	21.99	
2.48	31.02	27.78	38.72	53.73	3.58	8.01	0.9	0.28		
Ash composition analysis/%							Fusion temperature/°C		PS/μm/μm	
SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	CaO	MgO	Na ₂ O	K ₂ O	DT	ST	FT	37
53.81	35.79	3.58	1.420	0.49	0.62	1.15	> 1500	> 1500	> 1500	

ad is the dry base; HV is the high calorific value; and PS is the average particle size

Table 2. In the process of experiment, the temperature was first raised from ambient temperature to the setting temperature under nitrogen atmosphere. Next, the temperature was maintained constant and the atmosphere was switched to the setting atmospheres for gasification and combustion. The flow rate of total gas flow was set as 70 mL min⁻¹.

Kinetic method

The kinetic method of gasification and combustion used in this work is the same. Thus, only the kinetic method of gasification is introduced in detail. In TGA, the conversion ratio of char is defined as:

$$\alpha = \frac{M_i - M}{M_i - M_f} \tag{1}$$

where M_i is the initial mass of the sample during the gasification process, M_f is the final mass and M is the mass at certain time t .

The gasification rate of char can be described as:

$$\frac{d\alpha}{dt} = kP^m f(\alpha) \tag{2}$$

where $f(\alpha)$ is the differential expression of kinetic model equation, P denotes the partial pressure, m is the gasification reaction order and k represents the constant of the reaction rate and is usually described by the Arrhenius equation as:

$$k = k_0 \exp\left(-\frac{E}{RT}\right) \tag{3}$$

where k_0 is the pre-exponential factor (frequency factor), E is the activation energy and R is the universal gas constant ($R=8.314 \text{ J mol}^{-1} \text{ K}^{-1}$).

(1) Gasification reaction order m

When temperature T and conversion ratio of char α are constant, Eq. 4 can be obtained by taking logarithmic form of both sides of Eq. 2:

$$\ln\left(\frac{d\alpha}{dt}\Big|_{\alpha=c}\right) = m \ln(P_{\text{CO}_2}) + \ln(kf(\alpha)|_{\alpha=c}) \tag{4}$$

where c denotes the chosen value of α . Thus, based on Eq. 4, the plot of $\ln(d\alpha/dt)$ versus P_{CO_2} can fit to a straight line at the chosen value of α . The value of gasification reaction order m can therefore be obtained according to the slope of the line.

(2) Activation energy E

When partial pressure of CO_2 and conversion ratio of char α are constant, Eq. 5 can be obtained by taking logarithmic form of both sides of Eq. 2:

$$\ln\left(\frac{d\alpha}{dt}\Big|_{\alpha=c}\right) = -\frac{E}{RT} + \ln(k_0 P_{\text{CO}_2}^m f(\alpha)|_{\alpha=c}). \tag{5}$$

Thus, based on Eq. 5, the plot of $\ln(d\alpha/dt)$ versus $-1/RT$ can fit to a straight line at the chosen value of α . The value of activation energy E can therefore be obtained according to the slope of the line.

(3) Kinetic model equation $f(\alpha)$

The gasification reaction order m and activation energy E were obtained by iso-conversional method in steps 1 and 2. In step 3, the master plot method proposed by Gotor et al. [19] was used as a reference to predict the kinetic models of the gasification and combustion processes. The master plot

Table 2 Experimental conditions for gasification and combustion kinetics analysis of HN coal char

No.	Thermal treatment	Temperature/°C	Inert gas	Note
1	Gasification	1100	45%CO ₂ +55%N ₂	Isothermal TG
2	Gasification	1200	45%CO ₂ +55%N ₂	Isothermal TG
3	Gasification	1300	45%CO ₂ +55%N ₂	Isothermal TG
4	Gasification	1400	45%CO ₂ +55%N ₂	Isothermal TG
5	gasification	1300	55%CO ₂ +45%N ₂	Isothermal TG
6	Gasification	1300	65%CO ₂ +35%N ₂	Isothermal TG
7	Gasification	1300	75%CO ₂ +25%N ₂	Isothermal TG
8	Combustion	1100	5%O ₂ +95%N ₂	Isothermal TG
9	Combustion	1200	5%O ₂ +95%N ₂	Isothermal TG
10	Combustion	1300	5%O ₂ +95%N ₂	Isothermal TG
11	Combustion	1400	5%O ₂ +95%N ₂	Isothermal TG
12	Combustion	1300	10%O ₂ +90%N ₂	Isothermal TG
13	Combustion	1300	15%O ₂ +85%N ₂	Isothermal TG
14	Combustion	1300	21%O ₂ +79%N ₂	Isothermal TG

method used in this study is modified based on the method proposed by Gotor. The master plot method is based on the integral kinetic equation. The integral kinetic equation is defined as:

$$G(\alpha) = kt \quad (6)$$

where $G(\alpha)$ is the integral form of kinetic equation and k represents the constant of the reaction rate.

From the integral kinetic equation (Eq. 6), the following one using a reference at point $\alpha=0.5$ can be obtained:

$$G(\alpha|_{0.5}) = Kt|_{0.5}. \quad (7)$$

Dividing Eq. 6 by Eq. 7, one obtains:

$$\frac{G(\alpha)}{G(\alpha|_{0.5})} = \frac{t}{t|_{0.5}}. \quad (8)$$

The integral master plot method can be established by comparing the experimental plot of $t/t_{0.5}$ versus α with theoretical plots of $G(\alpha)/G(0.5)$ versus α using various kinetic models (Table 3). According to Eq. 8, the experimental value of $t/t_{0.5}$ is equal to the theoretical value of $G(\alpha)/G(0.5)$ at a fixed conversion α . Therefore, the reaction kinetic model

can be determined based on the comparison of the experimental and the theoretical master plots.

- (4) Kinetic parameters of gasification reaction: kinetic exponent n and pre-exponential factor k_0

As described in “Introduction” section, a complementary method of iso-conversional and model based was used in this work. Based on the above calculations, the gasification reaction order m and activation energy E were obtained by iso-conversional method. The kinetic model equation $f(\alpha)$ was obtained by the master plot method. The kinetic parameters of gasification reaction n and k_0 can be obtained by model-based method in the last step. Based on the known kinetic model equation $f(\alpha)$, kinetic exponent n can be obtained by the least square method [20, 21]. Based on Eq. 5, pre-exponential factor k_0 can be obtained according to the intercept of the line of $\ln(d\alpha/dt)$ versus $-1/RT$.

Result and discussion

Carbon conversion rate characteristics of high-AFT HN coal char

Figure 1 shows the carbon conversion rate and reaction rate curves of the gasification of HN coal char at different CO_2 partial pressures and temperatures. According to Fig. 1a, c, the carbon conversion rate increases significantly with increasing CO_2 partial pressure and temperature. The corresponding gasification reaction time of HN coal char is also shortened. According to Fig. 1b, d, the higher the CO_2 pressure and temperature, the higher the reaction rate. Gasification temperature has an important influence on the reaction rate of char gasification, and the increase in reaction temperature accelerates the gasification reaction. Figure 2 presents the carbon conversion rate and reaction rate curves of the combustion of HN coal char at different O_2 partial pressures and temperatures. The carbon conversion rate also increases significantly with increasing O_2 partial pressure and temperature. Combustion temperature has an important influence on the reaction rate.

Figure 3 shows the initial reaction rate curves of HN coal char at both gasification and combustion conditions. According to Fig. 3, the initial reaction rate curves of HN coal char at both gasification and combustion conditions can be divided into two zones at 1300 °C with different slopes. The activation energy of gasification and combustion reactions at lower-temperature region (1100–1300 °C) is higher than that at the higher-temperature region (1300–1400 °C). That is, at 1300 °C, the gasification and combustion processes are changed from the chemical reaction control (CRC) zone to the pore diffusion control (PDC) zone, where

Table 3 Expressions for the most frequently used reaction mechanisms

Symbol	Mechanisms	$f(\alpha)$	$G(\alpha)$
Reaction order models			
F_1	First order	$1 - \alpha$	$-\ln(1 - \alpha)$
F_2	Second order	$(1 - \alpha)^2$	$(1 - \alpha)^{-1} - 1$
F_3	Third order	$(1 - \alpha)^3$	$[(1 - \alpha)^{-2} - 1]/2$
F_4	Fourth order	$(1 - \alpha)^4$	$[(1 - \alpha)^{-3} - 1]/3$
Geometrical contraction models			
R_1	One dimension	1	α
R_2	Two dimensions	$2(1 - \alpha)^{1/2}$	$1 - (1 - \alpha)^{1/2}$
R_3	Three dimensions	$3(1 - \alpha)^{2/3}$	$1 - (1 - \alpha)^{1/3}$
Random nucleation and nuclei growth models			
A_2	Two dimensions	$2(1 - \alpha) [-\ln(1 - \alpha)]^{1/2}$	$[-\ln(1 - \alpha)]^{1/2}$
A_3	Three dimensions	$3(1 - \alpha) [-\ln(1 - \alpha)]^{2/3}$	$[-\ln(1 - \alpha)]^{1/3}$
A_4	Four dimensions	$4(1 - \alpha) [-\ln(1 - \alpha)]^{3/4}$	$[-\ln(1 - \alpha)]^{1/4}$
Nucleation models			
P_2	Power law, $n = 1/2$	$2\alpha^{1/2}$	$\alpha^{1/2}$
P_3	Power law, $n = 1/3$	$3\alpha^{2/3}$	$\alpha^{1/3}$
P_4	Power law, $n = 1/4$	$4\alpha^{3/4}$	$\alpha^{1/4}$
Diffusion models			
D_1	One-way transport	0.5α	α^2
D_2	Two-way transport	$[-\ln(1 - \alpha)]^{-1}$	$\alpha + (1 - \alpha) \ln(1 - \alpha)$

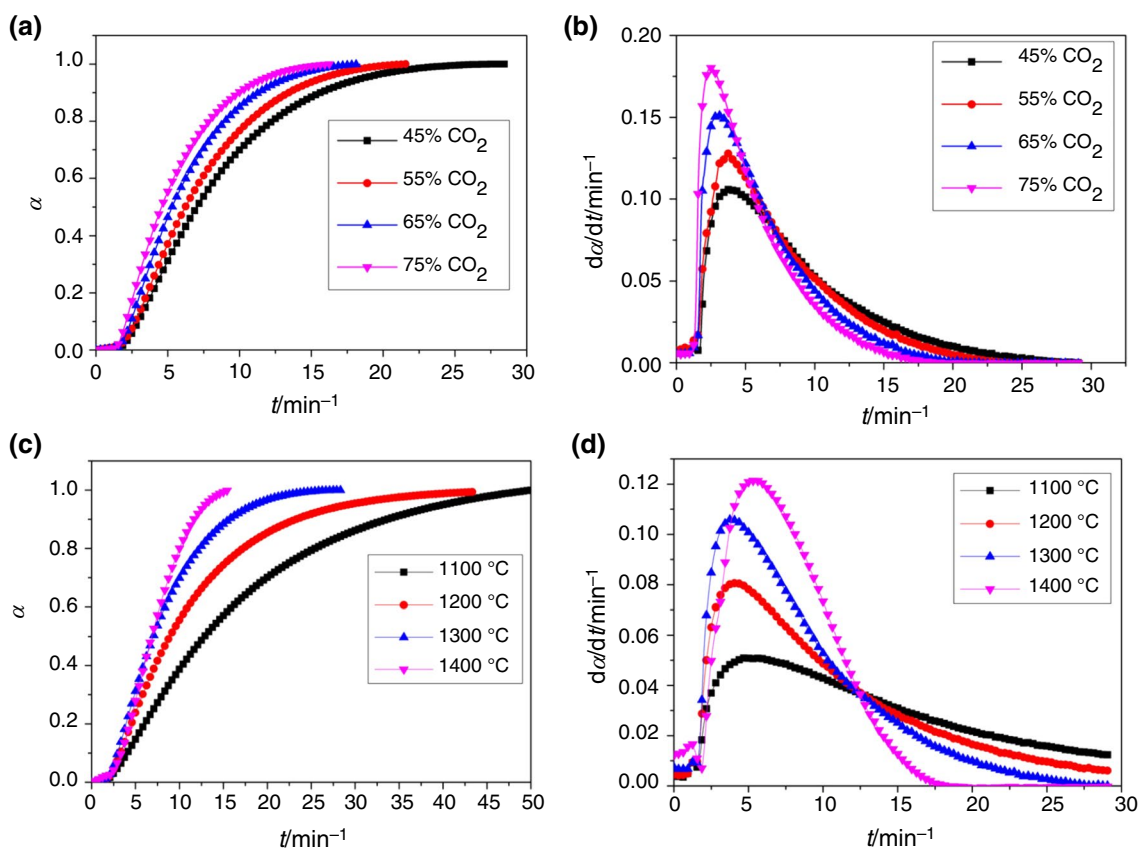


Fig. 1 Carbon conversion and reaction rate curves of the gasification of HN coal char: **a, b** at different CO_2 partial pressures (45%, 55%, 65% and 75%), **c, d** at different temperatures (1100 °C, 1200 °C, 1300 °C and 1400 °C). The data were recorded eight times per second

the dependence of reaction rate on temperature is less than that at chemical reaction control zone. Therefore, 1300 °C is recommended as the gasification temperature of the non-slugging EFGs system using high-AFT HN coal.

Determination of reaction order and activation energy

A complementary method of iso-conversional and model based is used in this work to analyze the gasification and combustion kinetics of HN coal char. Iso-conversional method is used to get gasification/combustion reaction order and activation energy. The detailed calculation methods are introduced in “Kinetic method” section. The plots for the determination of gasification/combustion reaction order and activation energy are illustrated in Fig. 4. The values of gasification/combustion reaction order and activation energy of HN coal char are listed in Table 4.

According to Fig. 4, these plots should be straight lines in theory as described in “Kinetic method” section. However, the plots in Fig. 4d are obviously not straight. This is because

the activation energy of gasification/combustion reactions at chemical reaction control zone (1100–1300 °C) is different from that at pore diffusion control zone (1300–1400 °C). Based on the data in “Carbon conversion rate characteristics of high-AFT HN coal char” section, the dividing point of the two zones is 1300 °C. Thus, the determination of combustion activation energy is based on two different zones as shown in Fig. 4d. Besides, Xiao et al. [22] analyzed the TG data of coal blends during combustion using iso-conversional method and the plots showed the same tendency. In our previous paper, the determination method of activation energy at different temperature regions was also adopted and it showed good accuracy [20, 21]. Moreover, based on Fig. 4b, the difference of gasification reaction activation energy between the two zones is not obvious. Therefore, only the average activation energy is analyzed for gasification reaction.

According to Table 5, the gasification and combustion reaction order is 9.2 and 9.3, respectively. The gasification reaction activation energy E of HN coal char is 80.74 kJ mol⁻¹. The combustion reaction activation energy

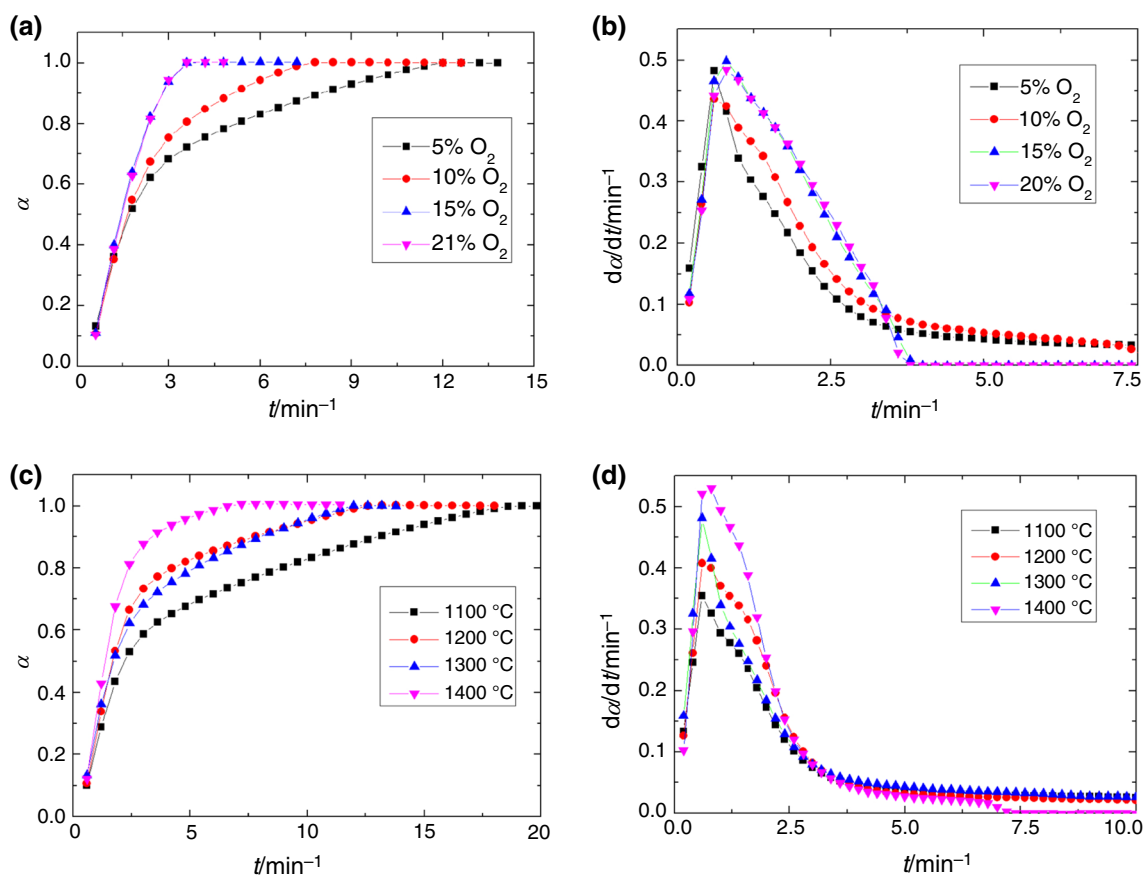


Fig. 2 Carbon conversion and reaction rate curves of the combustion of HN coal char: **a, b** at different O_2 partial pressures (5%, 10%, 15% and 21%), **c, d** at different temperatures (1100 °C, 1200 °C, 1300 °C and 1400 °C). The data were recorded eight times per second

E of HN coal char at chemical reaction control zone and pore diffusion control zone is 108.21 and 61.43 kJ mol^{-1} , respectively. In addition, according to Wang et al. [23], the activation energy of a coal during combustion was obtained as 80.92 kJ mol^{-1} using iso-conversional method. This value is close to the average value 84.82 kJ mol^{-1} in this study, which proves that the iso-conversional method is accurate for analyzing the activation energy of gasification and combustion.

Determination of kinetic model, kinetic exponent and pre-exponential factor with the complementary method

A complementary method of iso-conversional and model based is used in this work to analyze the gasification and combustion kinetics of HN coal char. The gasification/combustion reaction order and activation energy of HN coal char have been obtained by iso-conversional method. The remaining parameters are determined in this section, e.g.,

kinetic model, kinetic exponent and pre-exponential factor. Firstly, the kinetic model equation $f(\alpha)$ is obtained based on a modified master plot method. The principle of the method is introduced in “Kinetic method” section.

Theoretical plots of $G(\alpha)/G(0.5)$ versus α from various reaction models (Table 3) and experimental plots of $t/t_{0.5}$ versus α from experimental data are shown in Fig. 5. According to Fig. 5a, b, comparing the experimental plots ($t/t_{0.5}$ vs. α) with the theoretical plots [$G(\alpha)/G(0.5)$ vs. α], the kinetic model of gasification at different CO_2 partial pressures is nearly the same and is between A_1 and A_2 . The kinetic model of gasification at different temperatures is different, but still is between A_1 and A_3 . Thus, random nucleation and nuclei growth model is the kinetic model of gasification of HN coal char, i.e., $f(\alpha) = n(1 - \alpha) [-\ln(1 - \alpha)]^{1/n}$. As for combustion reaction, when the O_2 partial pressure is low, i.e., 5% and 10%, the kinetic model is found to be between F_1 and F_2 at each temperature. Thus, n th-order model is the kinetic model of combustion of HN coal char at low O_2 partial pressure, i.e.,

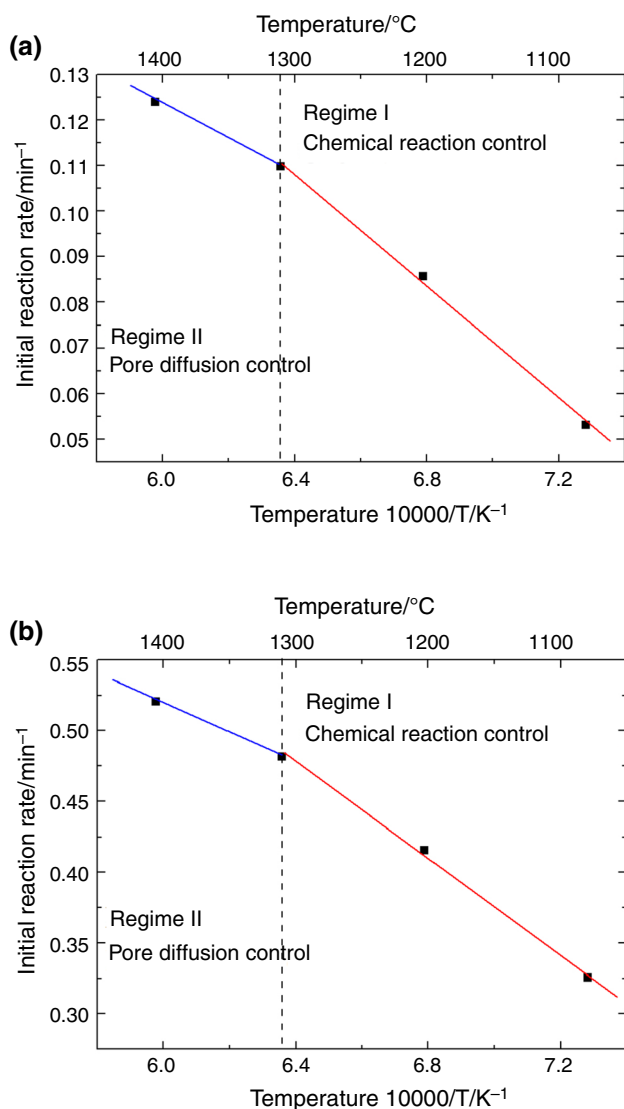


Fig. 3 Initial reaction rate curves of HN coal char: **a** gasification and **b** combustion

$f(\alpha) = (1 - \alpha)^n$. When the O₂ partial pressure is relatively high, i.e., 15% and 21%, the kinetic model is found to be between R₂ and R₃. Thus, geometrical contraction model is the kinetic model of combustion of HN coal char at relatively high O₂ partial pressure, i.e., $f(\alpha) = n \times (1 - \alpha)^{(n-1)/n}$. Comparing the kinetic model between gasification and combustion, it can be concluded that the temperature has a greater impact on the gasification kinetic model; however, the O₂ partial pressure has a greater impact on the combustion kinetic model.

Secondly, the kinetic exponent n and the pre-exponential factor k_0 need to be determined. As mentioned

in “Kinetic method” section, the two kinetic parameters can be obtained by model-based method. Based on the known kinetic model equation $f(\alpha)$ obtained by modified master plot method, kinetic exponent n is obtained by the least square method. Based on Eq. 5, pre-exponential factor k_0 is obtained according to the intercept of the line of $\ln(d\alpha/dt)$ versus $-1/RT$. Thus, the gasification/combustion reaction mechanism models, kinetic exponents and pre-exponential factors of HN coal char are obtained as shown in Table 5. The gasification/combustion reaction rate models of HN coal char were then obtained. Fine-tuning of kinetic parameters was performed to match experimental data, and the modified reaction rate models are listed in Table 6. Validation of the reaction rate equations in Table 6 with experimental data was conducted and is illustrated in Fig. 6 [24, 25]. Based on Fig. 6, the model prediction was in good agreement with the experimental data, which proved the predictive performance of the gasification/combustion reaction rate models of HN coal char proposed in this article.

Sensitivity and uncertainty analyses of this model were analyzed by using OAT method. That is, only one parameter was changed at a time, and parameters were analyzed according to the impact of parameter changes on simulation results. Reaction rate models of the gasification process of HN coal char at 45% CO₂ condition and combustion process at 5% O₂ condition were selected for sensitivity and uncertainty analyses. Only one parameter value was increased or decreased by 10%, and the effect of this change on the simulation results was calculated. Relative sensitivity (RS) was used to represent the sensitivity, and the calculation formula is as follows:

$$RS = \left| \frac{[y(x + \Delta x) - y(x)] / y(x)}{\Delta x / x} \right| \tag{9}$$

where x is a parameter value in the model parameter; Δx denotes the parameter change; and $y(x)$ and $y(x + \Delta x)$ represents the simulated output parameters before and after the change, respectively. The larger the RS value is, the more sensitive the parameter is; otherwise, it is insensitive. For gasification process, $RS(P_{CO_2})$ and $RS(T)$ are 0.920 and 0.005, respectively. For combustion process, $RS(P_{PO_2})$ and $RS(T)$ are 0.960 and 0.004, respectively. Moreover, the sensitivity and uncertainty analyses results are also illustrated in Fig. 7. It can be inferred that temperature has little influence effect on reaction rate. The partial pressures of CO₂ and O₂ are the main factors affecting the uncertainty of reaction rate models for gasification and combustion processes, respectively.

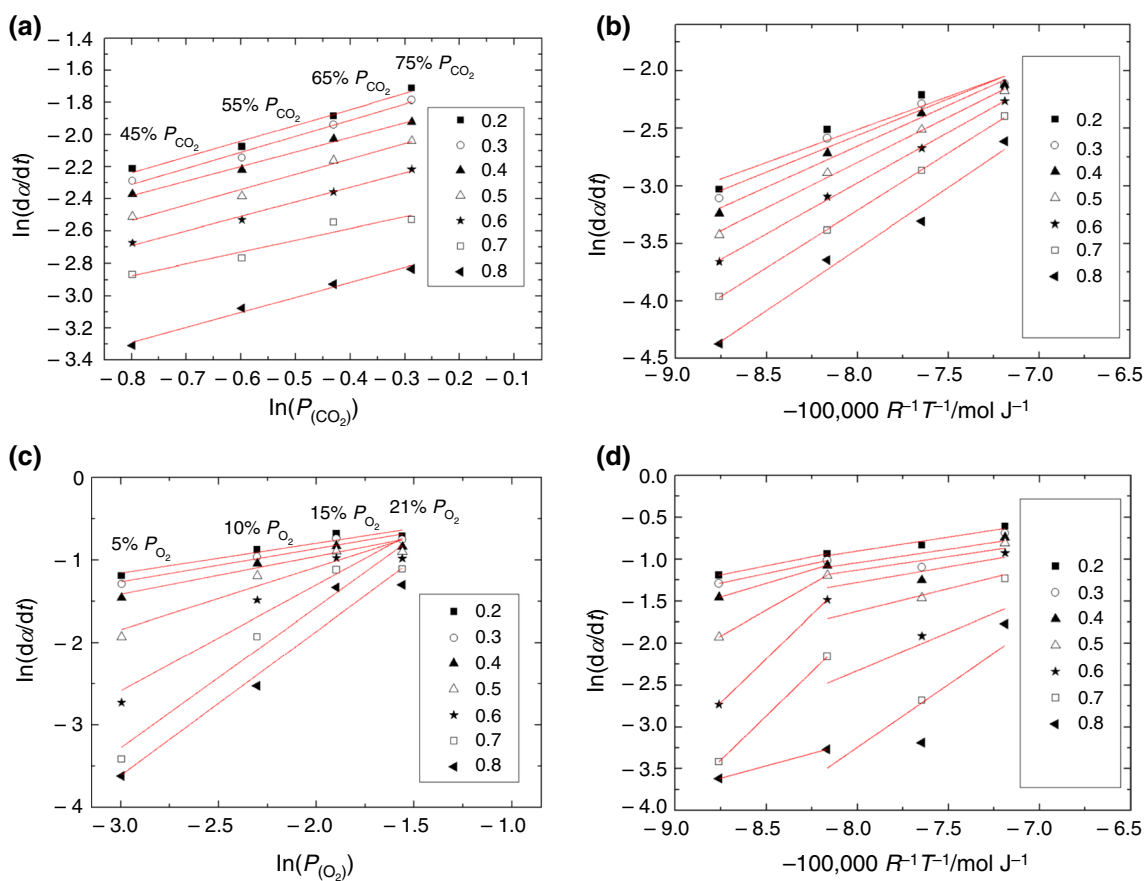


Fig. 4 Plots for the determination of reaction order and activation energy: **a, b** gasification process, **c, d** combustion process

Table 4 Gasification/combustion reaction order and activation energy of HN coal char

Carbon conversion α	Reaction order m		Activation energy $E/\text{kJ mol}^{-1}$		
	Gasification	Combustion	Gasification	Combustion	
				Reaction zone	Diffusion zone
0.2	0.98	0.36	57.26	43.41	33.22
0.3	1.00	0.40	63.61	46.01	32.36
0.4	0.91	0.46	71.15	64.47	32.29
0.5	0.95	0.75	78.77	123.84	37.33
0.6	0.90	1.29	88.05	209.64	54.06
0.7	0.73	1.71	99.49	211.28	90.72
0.8	0.93	1.75	106.83	58.84	150.03
Average	0.92	0.96	80.74	108.21	61.43

Table 5 Gasification/combustion reaction mechanism model, kinetic exponent and pre-exponential factor of HN coal char

Temperature/°C	Reaction mechanism model $f(\alpha)$		Pre-exponential factor k_0/min^{-1}
(a) Gasification reaction			
1100	$f(\alpha) = 1.26(1-\alpha)[- \ln(1-\alpha)]^{0.26/1.26}$		143.64
1200	$f(\alpha) = 1.33(1-\alpha)[- \ln(1-\alpha)]^{0.33/1.33}$		137.54
1300	$f(\alpha) = 1.53(1-\alpha)[- \ln(1-\alpha)]^{0.53/1.53}$		122.63
1400	$f(\alpha) = 2.17(1-\alpha)[- \ln(1-\alpha)]^{1.17/2.17}$		90.99
Temperature/°C	O ₂ partial pressure/%	Reaction mechanism model $f(\alpha)$	Pre-exponential factor k_0/min^{-1}
(b) Combustion reaction			
1100	5	$f(\alpha) = (1-\alpha)^{1.94}$	5537
1200	5	$f(\alpha) = (1-\alpha)^{1.34}$	2751
1300	5	$f(\alpha) = (1-\alpha)^{1.63}$	3855
1400	5	$f(\alpha) = (1-\alpha)^{0.90}$	1655
1300	10	$f(\alpha) = (1-\alpha)^{1.05}$	1011
1300	15	$f(\alpha) = 2.13 \times (1-\alpha)^{1.13/2.13}$	165
1300	21	$f(\alpha) = 2.47 \times (1-\alpha)^{1.47/2.47}$	96

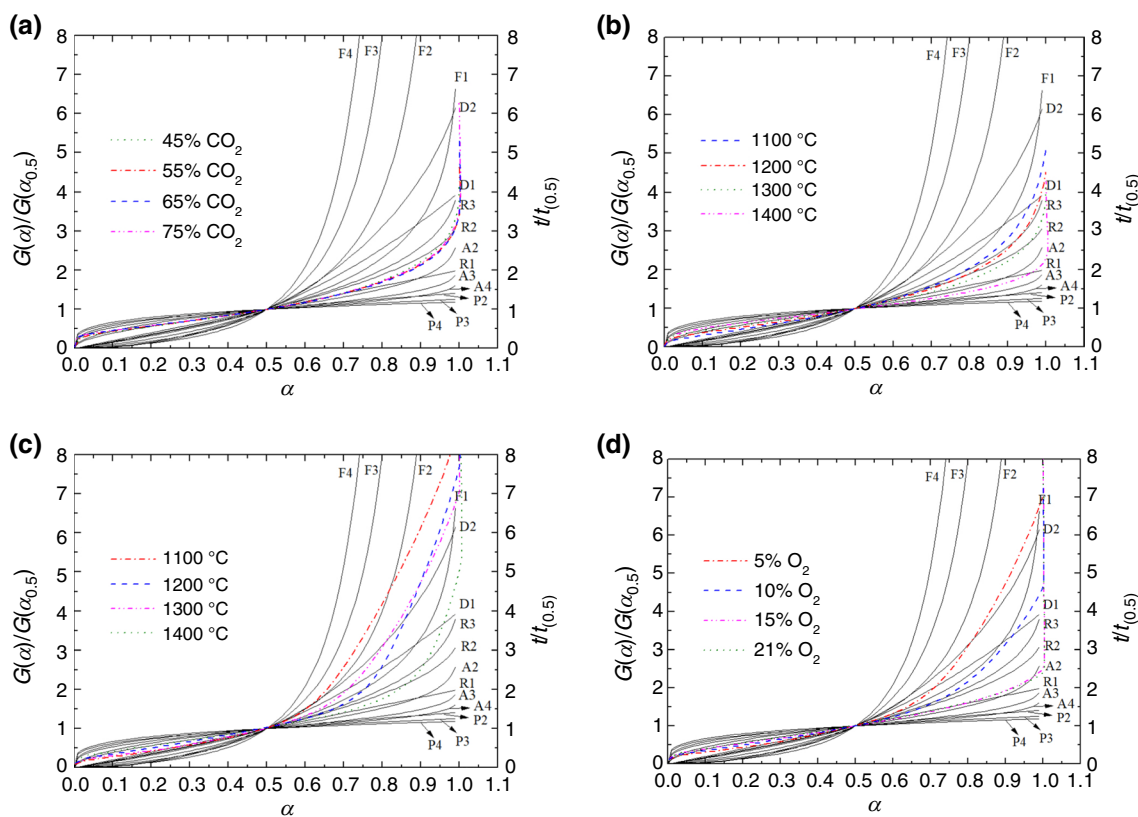
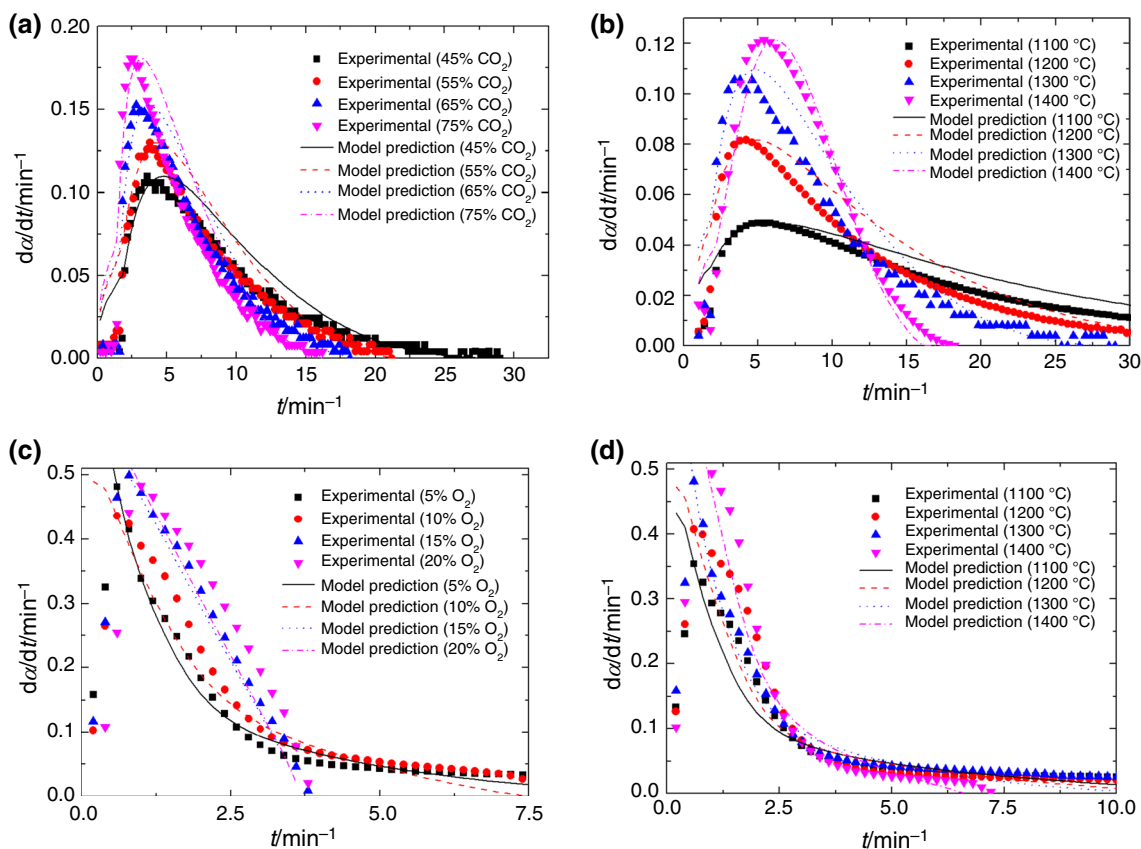


Fig. 5 Theoretical plots of $G(\alpha)/G(\alpha_{0.5})$ versus α from various reaction models (Table 3) and experimental plots of $t/t_{0.5}$ versus α from experimental data: **a, b** gasification process, **c, d** combustion process

Table 6 Gasification/combustion reaction rate model of HN coal char

Temperature/°C	Reaction rate model	
(a) Gasification reaction		
1100	$d\alpha/dt = 0.1383 \times \exp(-80.74/RT) \times P_{\text{CO}_2}^{0.92} \times 1.26(1-\alpha)[-\ln(1-\alpha)]^{(0.26/1.26)}$	
1200	$d\alpha/dt = 0.2341 \times \exp(-80.74/RT) \times P_{\text{CO}_2}^{0.92} \times 1.33(1-\alpha)[-\ln(1-\alpha)]^{(0.33/1.33)}$	
1300	$d\alpha/dt = 0.3067 \times \exp(-80.74/RT) \times P_{\text{CO}_2}^{0.92} \times 1.53(1-\alpha)[-\ln(1-\alpha)]^{(0.53/1.53)}$	
1400	$d\alpha/dt = 0.2806 \times \exp(-80.74/RT) \times P_{\text{CO}_2}^{0.92} \times 2.17(1-\alpha)[-\ln(1-\alpha)]^{(1.17/2.17)}$	
Temperature/°C	O ₂ partial pressure/%	Reaction rate model
(b) Combustion reaction		
1100	5	$d\alpha/dt = 7.792 \times \exp(-108.21/RT) \times P_{\text{O}_2}^{0.96} \times (1-\alpha)^{1.94}$
1200	5	$d\alpha/dt = 8.488 \times \exp(-108.21/RT) \times P_{\text{O}_2}^{0.96} \times (1-\alpha)^{1.34}$
1300	5	$d\alpha/dt = 10.83 \times \exp(-61.43/RT) \times P_{\text{O}_2}^{0.96} \times (1-\alpha)^{1.63}$
1400	5	$d\alpha/dt = 11.99 \times \exp(-61.43/RT) \times P_{\text{O}_2}^{0.96} \times (1-\alpha)^{0.90}$
1300	10	$d\alpha/dt = 4.496 \times \exp(-61.43/RT) \times P_{\text{O}_2}^{0.96} \times (1-\alpha)^{1.05}$
1300	15	$d\alpha/dt = 1.650 \times \exp(-61.43/RT) \times P_{\text{O}_2}^{0.96} \times 2.13 \times (1-\alpha)^{1.13/2.13}$
1300	21	$d\alpha/dt = 1.004 \times \exp(-61.43/RT) \times P_{\text{O}_2}^{0.96} \times 2.47 \times (1-\alpha)^{1.47/2.47}$

**Fig. 6** Validation of the reaction rate equations in Table 6 with experimental data: **a, b** gasification process, **c, d** combustion process

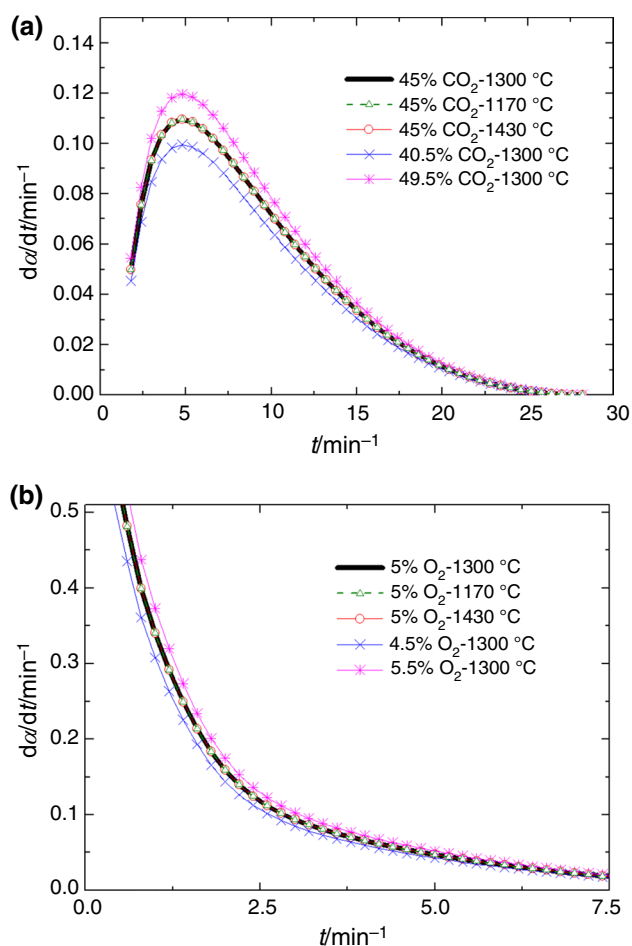


Fig. 7 Sensitivity and uncertainty analyses: **a** gasification process and **b** combustion process

Conclusions

In the present work, the gasification/combustion kinetics of a typical Chinese high-AFT coal char, Huainan coal char, are analyzed using a thermogravimetric analyzer. The carbon conversion rate and the gasification reaction rate increase significantly with increasing CO_2 partial pressure and temperature. Reaction temperature has a great impact on both the gasification and the combustion reaction rates, and the increase in reaction temperature accelerates the gasification/combustion reactions.

The initial reaction rate curves of HN coal char at both gasification and combustion conditions can be divided into two zones at 1300 °C. At 1300 °C, the gasification and combustion processes are changed from the chemical reaction control zone (1100–1300 °C) to the pore diffusion control zone (1300–1400 °C), where the dependence of reaction rate on temperature is less than that at chemical reaction control zone. Therefore, 1300 °C is recommended as the gasification

temperature of the non-slugging EFGs system using high-AFT HN coal.

Based on the isothermal method, a complementary method of iso-conversional and model based was used to analyze the gasification and combustion kinetics of HN coal char. Firstly, the gasification/combustion reaction order and activation energy of HN coal char are obtained by iso-conversional method. Then, the kinetic model equation $f(\alpha)$ is obtained based on a modified master plot method. The gasification kinetic model of HN coal char is random nucleation and nuclei growth model. The combustion kinetic model at low O_2 partial pressures (5%, 10%) and high O_2 partial pressures (15%, 21%) is n th-order model and geometrical contraction model, respectively.

Finally, the kinetic exponent n and the pre-exponential factor k_0 are obtained by model-based method. Based on the known kinetic model equation $f(\alpha)$, kinetic exponent n is obtained by the least square method. Based on Eq. 5, pre-exponential factor k_0 is obtained according to the intercept of the line of $\ln(da/dt)$ versus $-1/RT$. The results of this work provide the useful data for designing the non-slugging EFGs using high-AFT coals.

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