Fuel 314 (2022) 122772

Contents lists available at ScienceDirect

Fuel

journal homepage: www.elsevier.com/locate/fuel

Full Length Article

Ignition predictions of isolated coal particles by different ignition criteria and devolatilization models

Wantao Yang, Yang Zhang, Bing Liu, Kailong Xu, Hai Zhang *

Key Laboratory for Thermal Science and Power Engineering of Ministry Education, Department of Energy and Power Engineering, Tsinghua University, Beijing, China

ARTICLE INFO

Keywords:
Ignition
Isolated coal particles
Ignition criterion
Devolatilization model
Microgravity experiments

ABSTRACT

The prediction accuracy of coal ignition characteristics depends on the sub-model selections. A detailed modeling study on the influences of ignition criteria and devolatilization models on the ignition characteristics of isolated coal particles is conducted using a one-dimensional transient ignition model. The assessed ignition criteria include the thermal explosion theory (TET), the transient adiabatic criterion (TAC) and the flammability limit criterion (FLC), while the assessed the devolatilization models include the chemical percolation devolatilization (CPD) one and two competing reaction (TCR) one. Under each combination, the ignition characteristics under different oxygen concentration, particle size, and surrounding temperature are studied. The prediction results are compared with microgravity experimental data obtained from the 3.6 s drop tower in National Microgravity Laboratory Center of China (NMLC). Modeling results reveal that the particle center temperature is more reasonable to be used as the characteristic temperature in the ignition study. When devolatilization process is described by CPD model, for homogenous ignition FLC is more accurate to predict ignition temperature and time than TAC at a higher X_{O2} and a high T_w, while TAC is more accurate to predict ignition temperature at a large particle size. Using FLC, against TAC, the transient of ignition mode from homogenous to combined happens at a ~ 80 K higher temperature and ~ 50 μm larger particle size, while that from combined to heterogenous happens at 250 μm rather than 400 μm. When FLC is used as the ignition criterion, selection of devolatilization model has more notable effect on the prediction of ignition temperature and time. Furthermore, the combination of FLC and CPD is more accurate to predict ignition temperature and time at a higher X_{O2}. Two diagrams are respectively given to guide the selection the ignition criterion and identify the ignition mode at a wide range of conditions. In addition, the mechanisms of the associated discrepancy are discussed.

1. Introduction

Ignition is the initiation step in coal particle combustion. The ignition characteristics, including the ignition delay time (τ_i), ignition temperature (T_i), and ignition mode of isolated coal particles are important to describe the ignition process and the necessary input in CFD modelling for coal combustion as well [1–5]. Even though coal combustion is limited due to the carbon neutral requirement, it will continue to play an important role in power generation in the next a few decades. For example, in China, the coal firing currently counts more than 70% of the total power generation and is expected to keep more than 15% of the total power generation in 2060 when carbon neutral is realized. Increasing the coal combustion efficiency and well controlling the coal process is indeed benefit for reducing carbon emission. Thus, the development of digital coal-fired power plants which is based on CFD modelling of coal combustion in a boiler becomes increasingly demanded, while the CFD modelling needs the support of the accurate ground models, including ignition models of an isolated coal particle.

The ignition of an isolated coal particle has been studied for decades and several ignition models have been developed [1–14]. The existing models can be divided into steady state ones and transient ones. Though the steady state models can predict T_i, i.e., the temperature of the coal particle when ignition occurs, and is convenient to study the effects of particle size (d_p), oxygen concentration (X_{O2}) and furnace temperature (T_w) on T_i [1–3], they cannot well predict τ_i, the period from the moment when the coal particle is put into a hot environment to the moment when ignition occurs. Thus, to more accurately predict τ_i, some transient models were developed [6–13]. No matter in which kind of ignition model, the criterion to justify whether ignition occurs and the description of the release of volatile matter (VM) are core sub-models. Different ignition criterion and devolatilization model could result in different ignition characteristics.

There are three ignition criteria reported in the previous studies. The

* Corresponding author.

https://doi.org/10.1016/j.fuel.2021.122772
Received 17 August 2021; Received in revised form 25 October 2021; Accepted 28 November 2021
Available online 9 December 2021
0016-2361/

Nomenclature

Notations

A	Pre-exponent factor
c_0	Number of intact bridges
d	Particle size/mm
E	Reaction activation energy
f	Mass fraction
L_0	Fraction of intact bridges
MW_{cl}	Molecular weight per cluster
MW_{δ}	Molecular weight per side-chain
r	Distance/mm
r^*	Dimensionless distance
R	Ideal gas constant
T	Temperature/K
X	Mole fraction
Y	Yield factor
τ	Time/s
TET	Thermal explosion theory
TAC	Transient adiabatic criterion
FLC	Flammability limit criterion
CPD	Chemical percolation devolatilization
TCR	Two competing reaction
c	Center
f	Flame front
hetero	Heterogeneous ignition
homo	Homogeneous ignition
i	Ignition
p	Particle
py	Pyrolysis
v	Volatile matter
$\sigma + 1$	Coordination number

classic one is the thermal explosion theory (TET) used to prediction the heterogeneous ignition [1,5]. According to TET, ignition occurs as the heat generation on particle surface is greater than the heat released to the environment. Modellings adopting such a criterion can well predict the occurrence of heterogeneous ignition at a given T_w and the variation trends of T_i with respect to T_w [6,8]. Judged by TET criterion, if the calculated particle temperature history curve shows an inflection point, shown in Fig. 1a, then heterogeneous ignition occurs and the time from initial heating to the inflection point is τ_i [5]. However, TET criterion is invalid to judge whether and when ignition occurs in the gas-phase. Accordingly, to predict homogeneous ignition, two other ignition criteria, i.e., the transient adiabatic criterion (TAC) and flammability limit criterion (FLC) were purposed [7,9].

When TAC is adopted, homogeneous ignition is identified to occur in the gaseous reaction zone around the particle by comparing the heat generation with the heat loss. On the non-monotonous radial temperature profile, a flame is regarded to exist at the peak temperature, as shown in Fig. 1b. The time from the initial heating to appearance moment of the peak temperature is τ_i [7]. FLC adopts the flammability limit concept of a premixed mixture, and assumes that oxygen and volatiles are diffusing into each other, forming a layer of combustible mixture. Radial VM composition distribution is calculated till ignition occurs. Shown in Fig. 1c, homogeneous ignition occurs when the accumulated VM meets the flammability limit at certain local gas temperature and X_{O2} [9]. The time from the initial heating to the commence of ignition is τ_i.

However, the predicted ignition characteristics or even the variation trends are inconsistent or even opposite by adopting different ignition criterion. For example, the ignition models with either TAC or FLC correctly predicted that as X_{O2} increases ignition mode converts homogeneous to heterogeneous, but in term of the variation τ_i with X_{O2} the model using FLC predicts a smooth trend while the model using TAC shows a sudden drop [6]. The transition of ignition mode is attributed to the competition of reaction rates between heterogeneous char and homogeneous volatiles [2] or the relative time scales of the volatile evolution and heterogeneous surface reaction [10]. Compared with the experimental results, the model with FLC is more accurate than the one with TAC in predicting the variation trend of T_i with X_{O2} [6,13].

Studies also found that the models with improper ignition criterion incorrectly predict ignition behaviors under different d_p's and T_w's [6–8]. On one hand, experimental results showed that the homogeneous ignition becomes dominant, and T_i decreases while τ_i increases when d_p is rather large [6,14]. On the other hand, the model with TET only correctly predicts the variation trend of T_i with d_p but fails to predict that of τ_i with d_p [15,16]. As d_p increases to a certain value, both T_i and τ_i are predicted to be smaller [17,18]. More recent studies found the contradiction is attributed to the intra-particle thermal conduction, which decreases the overall particle temperature (T_p) as the coal particles is in mm-sized and above [6,19,20]. By using the center temperature (T_c) rather than the surface temperature (T_s) as the characteristic temperature, the variation trends of T_i and τ_i with d_p can be correctly predicted [6,21]. Moreover, modelling results showed that both T_s and T_c increase with T_w by using TET while the variation trend is opposite by using TAC [6,8,21]. However, experimental results only show T_c increases with T_w [21]. The contradict results show that the variation and interaction of operation parameters on T_c and ignition mode still need to be further investigated. Also, a guidance to properly select criterion among the TET, TAC and FLC in a wider range of operating conditions is desired.

Besides the ignition criterion, the devolatilization description plays important role in the ignition modelling as well. Different description of

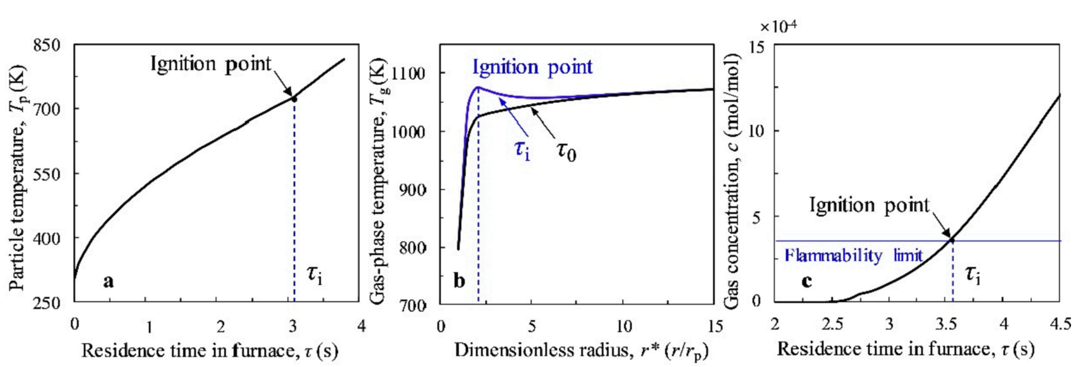

Fig. 1. The ignition occurrence identified with different ignition criterion in the modeling (a: TET, b: TAC, c: FLC).

the devolatilization process can result in remarkable difference in pyrolysis delay time, VM release rate, the particle temperature, and thereby different ignition characteristics [6,11,12]. Currently, there are two most commonly used devolatilization models; one is the two-step chemical kinetic (TRC) model and the other is chemical percolation devolatilization (CPD) model. In TRC model, devolatilization rate is described by two competing kinetic steps with different activation energies, one step prevailing at low temperatures and the other step prevailing at high temperatures [22]. The CPD model is a network devolatilization model, assuming that coal macromolecular structure can be approximately described by aromatic clusters connected by aliphatic bridges. It includes rates for bridge breaking and side chain release, percolation lattice statistics to relate the number of broken bridges to the distribution of clusters that detach from the lattice, vapor–liquid equilibrium to determine the sizes of detached clusters that vaporize to form tar, and crosslinking of non-vaporized detached fragments that become part of the char [23]. CPD model well describes the composition and the evolution of intermediates of the VM in a certain range of temperature and heating rates. It was found both TRC and CPD models well predict τ_i under various coals, heating rates and temperature. However, the existing studies have been done by using the combination of TET and TAC only, and only in a small range of X_{O2}'s. In another word, the coupling effect of devolatilization model with ignition criteria still need to be fully assessed.

Consequently, in this work, three ignition criteria and two devolatilization models are respectively adopted in a 1-D transient ignition model with the consideration of intraparticle thermal conduction for isolated coal particles. Under each combination, the ignition characteristics under various X_{O2}'s, d_p's and T_w's are studied. The predictions are compared with the data obtained at microgravity (μg) experiments. Two diagrams are respectively given to guide the selection the ignition criterion and identify the ignition mode at a wide range of conditions (Fig. 2).

2. Modelling approach

Consistent with the μg experimental settings introduced in the latter section, an isolated coal particle is located in an environment with a preset T_w and X_{O2}. It is heated up by thermal radiation from the wall and thermal conduction from the surrounding gas. Natural convection is neglected and the particle is assumed to 1-D along the radial direction.

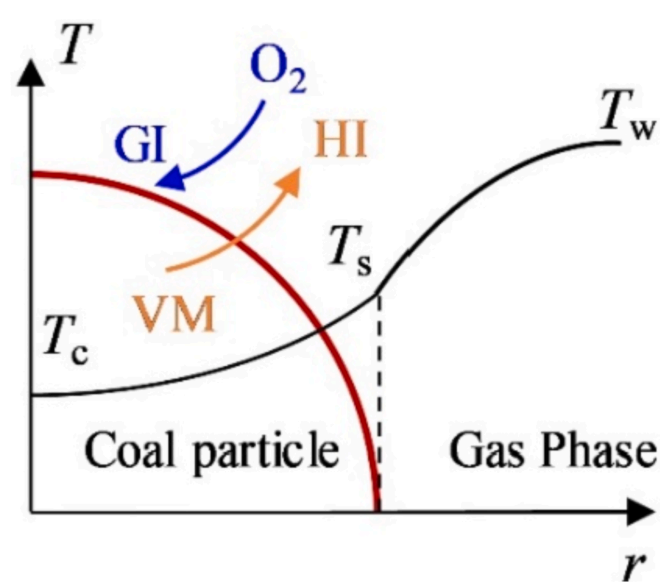

Fig. 2. The physical model for ignition of single c oal particle with intraparticle temperature gradient (GI: Heterogeneous ignition, HI: Homogeneous ignition).

The devolatilization is assumed to be uniform and spherically symmetric. Intraparticle thermal conduction is considered. The coal properties are consistent with those in the experiments. The governing equations and boundary conditions are can be found in previous work [6].

Datong bituminous coal was used in the experiments and its proximate and ultimate analyses are given in Table 1.

TCR and CPD models are respectively used to described the coal devolatilization. When TCR is adopted, the devolatilization rate is expressed at a given heating rate in Eq. (1).

$$\frac{d(V)}{dt} = \left(Y_1 A_1 e^{-\frac{E_1}{RT}} + Y_2 A_2 e^{-\frac{E_2}{RT}}\right) \quad (1)$$

The combustible light gas components in CPD are assumed to be CH_4, H_2 and CO.

The parameters in CPD and TCR models are listed in Table 2, and the details to obtain these parameters can be referred in the literatures [6,24].

As introduced in the previous sections, TET is used to identify the heterogeneous ignition, while TAC and FLC are adopted to judge the homogeneous ignition.

3. Experiments

At microgravity (μg), the effect of buoyancy is minimized [13,14,25] and thus the one-dimensional (1-D) assumption of ignition and combustion of the isolated single coal particles can be more reasonably, consistent to that in the modelling. In this study, the μg experiments were carried out in the drop tower at the National Microgravity Laboratory Center of China (NMLC), with μg time of 3.6 s. A schematic diagram of the experimental system is shown in Fig. 3. More details of experimental system and procedures can be referred to our previous studies [13].

The coal particle was ~2.0 mm in size, nearly spherical. To measure the center temperature, a fine bare-wired K type thermocouple was installed in the center isolated coal particles. The thermocouple wire diameter was 0.125 mm with a joint diameter of 0.25 mm. The measurement error of T_i was ~20 K [21].

The oxidizer gas was a mixture of O_2/N_2, with X_{O2} set to 21%, 30%, 40% and 50% respectively. The furnace was pre-heated to 1123 K.

4. Results and discussion

4.1. Prediction on dependency of T_i and τ_i on X_{O2}, d_p and T_w

Figure 4 shows the radial gas temperature (T_g) profiles calculated by the ignition model with TAC at three X_{O2}'s and three d_p's. The devolatilization process is described by CDP model. The flame front temperature (r_f) keeps constant as X_{O2} changes, indicating that the heat generation and loss nearly equal in the reaction zone [7]. The slight decrease in T_i might be attributed to the change of thermal conductivity under different X_{O2}'s. Shown in Fig. 4b, in the air, a smaller coal particle leads to a lower heat loss and then a higher T_g in reaction zone, thereby a higher T_i. For FLC, the flammability limit when $X_{O2} = 50\%$ is two orders of magnitude lower than that of 21%, leading to decreasing trend of T_i with increasing X_{O2}.

From the radial gas temperature distributions, T_i andτ_i can be

Table 1
The proximate and ultimate analyses of the test coal.

Proximate analysis, wt.% (air dry basis)				
Volatile matter	Ash	Moisture	Fixed carbon	
27.43	12.54	2.73	57.27	
Ultimate analysis, wt.% (air dry basis)				
Carbon	Hydrogen	Oxygen	Nitrogen	Sulfur
71.82	3.84	5.65	0.90	2.52

Table 2
Chemical structure parameters and two-step reaction parameters in modelling.

Chemical structure parameters					
MW_{cl}	MW_{δ}	L_0		$\sigma+1$	c_0
27.43	12.54	2.73		25.1	291.6
Two-step reaction parameters					
A_1	A_2	E_1/R	E_2/R	Y_1	Y_2
2×10^5 s^{-1}	1.3×10^7 s^{-1}	1.26×10^4 K	2.01×10^4 K	0.3	1.0

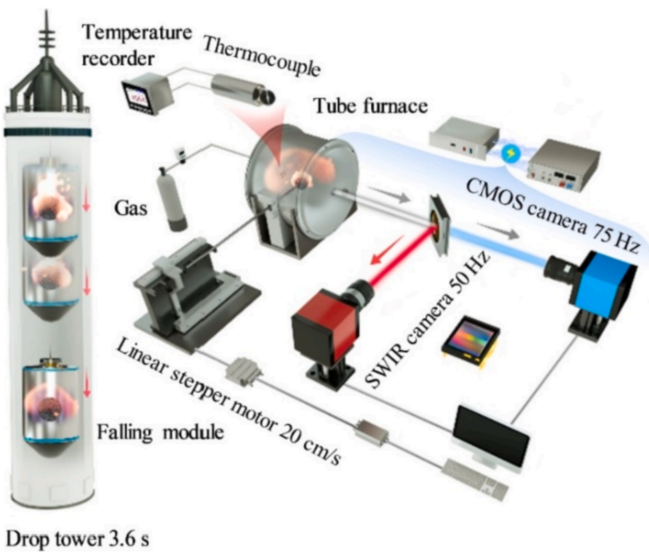

Fig. 3. The scheme of the microgravity experimental system.

obtained. Shown in Fig. 5, measured T_i andτ_i present a noticeably decreasing trend with the increasing X_{O2}. For a bituminous coal, only FLC and TAC are used. When FLC criterion is adopted, the variation trend is correctly predicted. However, when TAC is used, the predicted T_i and τ_i are nearly independent of X_{O2}. The variation trends of T_c by FLC and TAC are consistent with that of T_s reported in literature, while the discrepancy between TAC and FLC is more significant for a larger d_p.

Shown in Fig. 6a, the predicted variations of T_i with d_p by the ignition model with TAC agree well with the measured data. Although a similar decreasing trend can be predicted by the ignition model with FLC, the predicted values are ~80 K lower than the measured ones. At a lower T_w, e.g. 923 K, the predicted T_i's by either criterion are nearly the same. When $T_w > 973$ K, the results calculated by FLC have obvious deviations from the experimental values. On the other hand, shown in Fig. 6b, τ_i's predicted by TAC and FLC are consistent and agree well with the experimental results.

Figure 7 shows that variation of T_i with T_w predicted by the ignition model with FLC ignition criterion decreases more rapidly than that of measured one, especially when $T_w > 973$ K. The difference reaches ~100 K when $T_w = 1123$ K. The discrepancy may be caused by over-predicted kinetic parameters and physico-chemical constants [13]. By comparison, both T_i and τ_i display a decreasing trend with respect to T_w and agree well with the predicted values by TAC.

The results of Figs. 6 and 7 showed that both TAC and FLC have their own limitations in accurate prediction of T_i, especially under the coupling interaction effect of multiple factors. To assess the causes, Fig. 8 depicts the temporal variations of the particle center temperature (T_c) and released volatile matter fraction (f_{vol}) under different X_{O2}'s. It can be seen that the VM release rate and particle temperature history are nearly the same at different X_{O2}'s, indicating that X_{O2} does not remarkably change the devolatilization and heating rate, thereby T_i. The devolatilization time (τ_{py}) increases and particle heating rate decreases with increasing d_p, leading to longer time to reach the flammability limit in FLC or to reach the thermal peak in TAC, thereby an increasing τ_i. Meanwhile, smaller particles are subjected to a higher heating rate, leading to a higher T_i when f_{vol} meets the flammability limit. This could well explain why the experimental data show that τ_i increases but T_i decreases with respect to d_p. The effects of T_w and d_p onτ_{py} and particle heating rate cannot ignored in ignition prediction.

4.2. *Prediction on dependency of ignition mode on d_p and T_w*

Figure 9 displays the τ_i's predicted by using TAC, FLC and TET under different T_w's and d_p's. If the calculated homogeneous τ_i ($\tau_{i,\ homo}$) is shorter than the heterogeneous one ($\tau_{i,hetero}$), the ignition mode is homogeneous and vice versa [6]. At a lower T_w, $\tau_{i,hetero}$ is always higher than $\tau_{i,homo}$, indicating that ignition mode is homogeneous. As T_w increases, $\tau_{i,hetero}$ decreases faster than $\tau_{i,homo}$ and they converge gradually, resulting in the combined ignition mode. In addition, $\tau_{i,homo}$ predicted by FLC is smaller than that predicted by TAC at a high T_w.

Both $\tau_{i,hetero}$ and $\tau_{i,homo}$ keeps increasing with d_p. For small particles, the calculated $\tau_{i,hetero}$ is lower than $\tau_{i,homo}$, leading to a heterogeneous ignition. As d_p increases, $\tau_{i,hetero}$ gradually increases and finally exceeds $\tau_{i,homo.}$ As a result, ignition mode changes from heterogeneous to combined and then to homogeneous. For small particles, $\tau_{i,homo}$ predicted by TAC slightly higher than $\tau_{i,hetero}$, and the heterogeneous ignition becomes and combined ignition at d_p ≈75 μm. As d_p increases from 250 μm to 400 μm, $\tau_{i,homo}$ becomes remarkable higher for TAC against FLC.

Figure 10 depicts the ignition modes of isolated coal particles under different d_p's and T_w's in the air combustion. Generally speaking, when TAC or FLC is used, heterogeneous ignition is more likely to occur for small coal particles and homogeneous ignition is in favor of large coal particles. When the heating rate or T_w is high enough, combined ignition

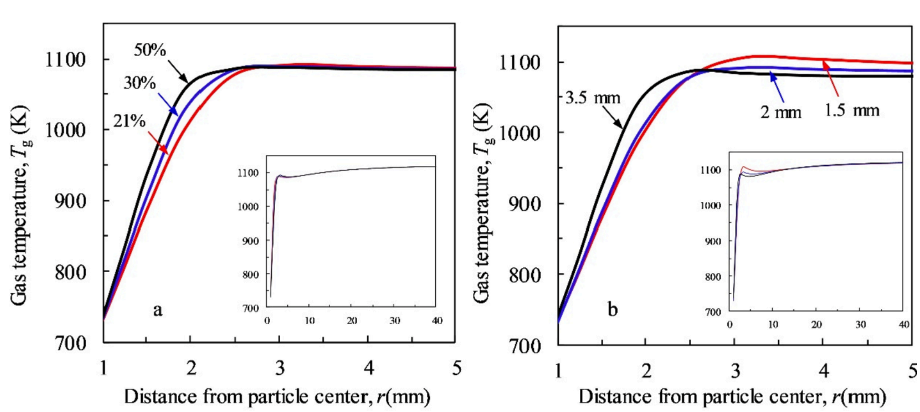

Fig. 4. The radial gas temperature distribution around a coal particle at different X_{O2} or d_p when $T_w = 1123$ K (a: $d_p = 2$ mm, b: $X_{O2} = 21\%$) (The embedded small figure refers to the gas temperature distribution in the gas space extending further to 40 r_0).

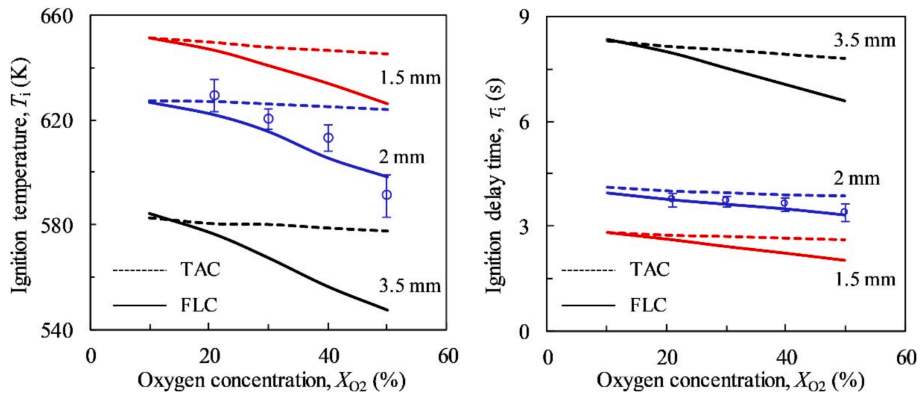

Fig. 5. Variations of the calculated and measured τ_i and T_i with X_{O2} of isolated coal particles at different d_p (T_w = 1123 K).

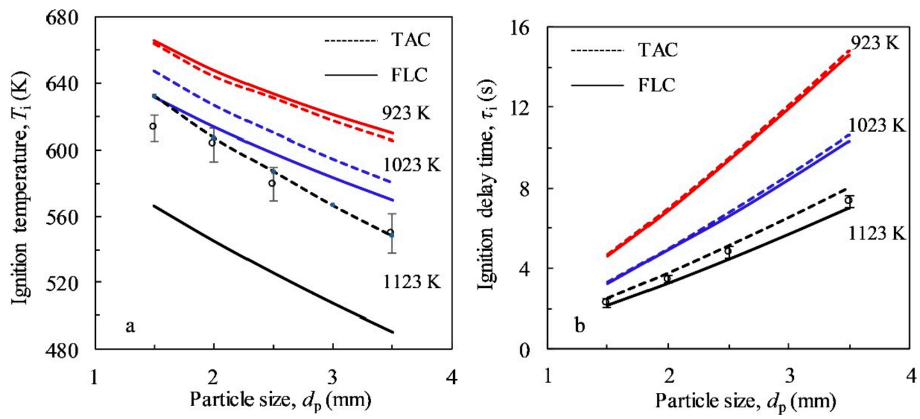

Fig. 6. Variations of the calculated and measured τ_i and T_i with d_p of isolated coal particles under T_w's (X_{O2} = 21%).

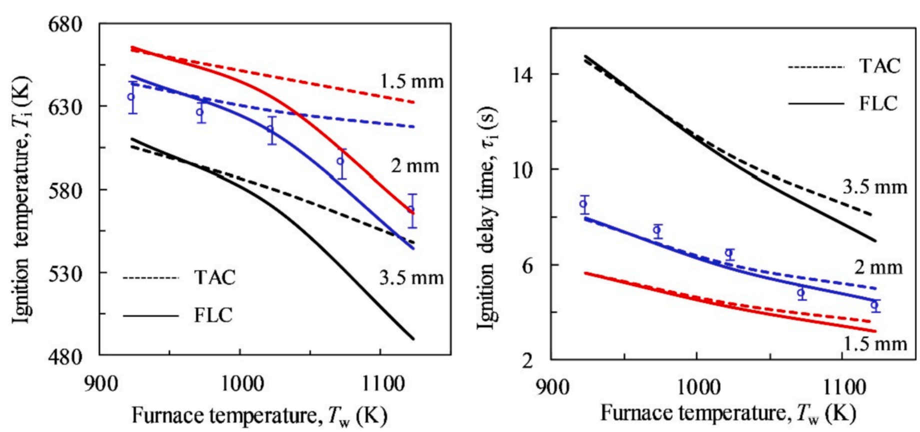

Fig. 7. Variations of the calculated and measuredτ_i and T_i of isolated coal particles with T_w at different d_p (X_{O2} = 21%).

occurs. The critical T_w at which ignition mode changes increases from 973 K to 1073 K for TAC, because the predicted $\tau_{i,homo}$ is shorter by FLC. In other words, the time to reach the flammability limit is shorter than to attain the thermal peak with respect to T_w. Critical d_p slightly decrease from 150 μm to 100 μm using FLC because τ_i is less sensitive to d_p than using TAC.

Since ignition mode must be distinguished before the selection of ignition criterion, hence, a diagram for the criterion selection in a wide range of X_{O2}'s, d_p's and T_w's is given in Fig. 11. The operation parameters cover those used in fluidized bed boilers [26], pulverized boiler, moderate or intense low-oxygen dilution (MILD) combustion and oxy-fuel combustion [27].

Illustrated in Fig. 11, the diagram is divided into three zones, one is the bottom zone regarding to the interaction of X_{O2} and d_p, one is the right zone regarding to the interaction of T_w and X_{O2}, and another is the left zone regarding to the interaction of d_p and T_w. At the bottom zone, heterogeneous ignition occurs when X_{O2} exceeds 40%, in which TET is suggested to be selected. The critical d_p increases as X_{O2} decreases, which agree with the results reported in literature [6]. Besides, FLC is more accurate to predict the homogenous ignition characteristics of isolated coal particles with respect to X_{O2}. Depicted in the right zone, homogeneous ignition tends to occur at a condition that the T_w is lower than 1273 K. Both FLC and TAC can be used for the prediction of T_i with further limitation of T_w lower than 973 K; otherwise, only TAC makes

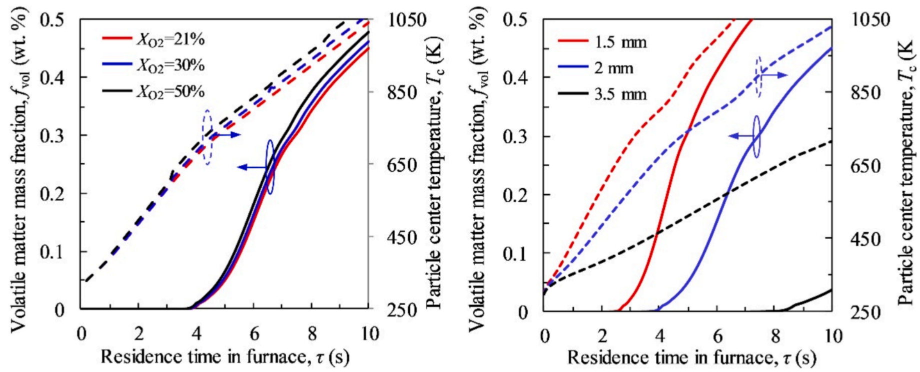

Fig. 8. The temporal variations of particle center temperature and volatile matter fraction under different X_{O2}′s (a: $d_p = 2$ mm, $T_W = 1123$ K) and d_p's (b: $X_{O2} = 21\%$, $T_W = 1123$ K).

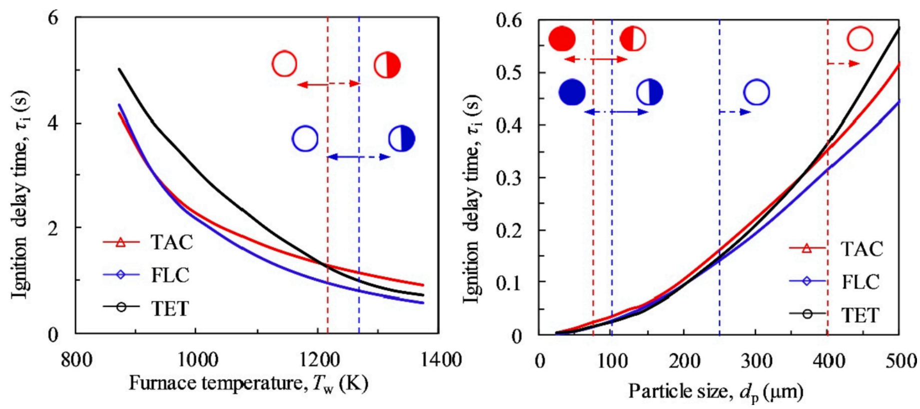

Fig. 9. Variations of ignition mode and τ_i predicted with TAC and FLC under different T_w's (a; $d_p = 2$ mm, $X_{O2} = 21\%$) and d_p's (Solid point: heterogeneous ignition, Hollow point: homogeneous ignition, Semi solid point: combined ignition, $T_w = 1123$ K, $X_{O2} = 21\%$).

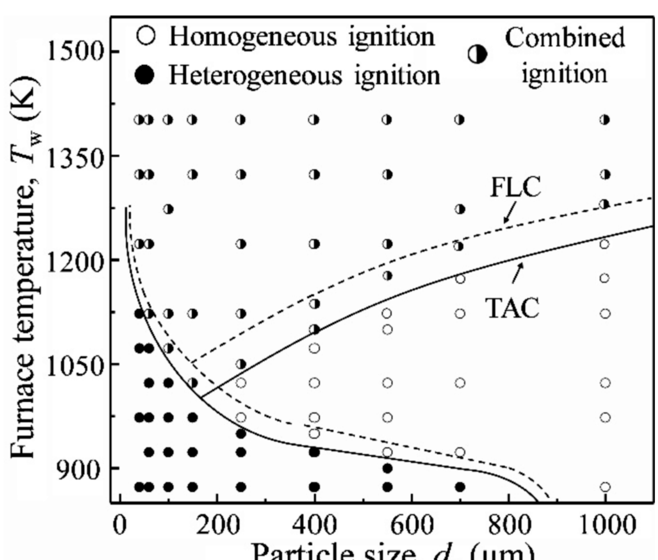

Fig. 10. A diagram to identify the ignition mode of isolated coal particles under different d_p's and T_w's in the air combustion.

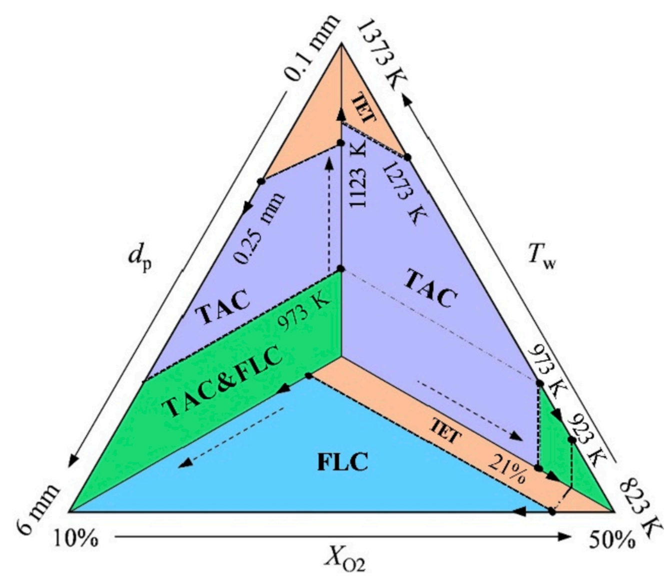

Fig. 11. A diagram to selection of ignition criteria in ignition model for accurate prediction of T_i in under the interaction of different X_{O2}′s, d_p's and T_w's.

available predictions. Coupled with the effect of X_{O2}, the critical T_w changes from 973 K to 923 K when X_{O2} increases from 21% to 40%. Shown in the left zone, under the condition of 1123 K, TET is suggested to be selected under these conditions when d_p is less than 0.25 mm. Due to the interaction of d_p and T_w, the critical d_p for TET increases with T_w. Both FLC and TAC are reasonable for ignition prediction under different d_p, but FLC is not available to assess interacted effect when T_w exceeds 973 K.

4.3. Coupling effect of ignition criteria and devolatilization model on ignition prediction

Figure 12 depicts the effects of different combination of ignition criteria and devolatilization model on ignition temperature and delay time of isolated coal particles. It can be seen that the variation trends of T_i and τ_i with respect to X_{O2}'s display a similar downward variation trend regardless of CPD or TCR devolatilization models, but the values of TCR model are remarkably higher. When FLC is used as the ignition criterion, the difference in the predicted T_i and τ_i is quite noticeable between CPD and TCR. While TAC is used as the ignition criterion, the difference is much less. The results indicate that when FLC is used as the ignition criterion, the selection of devolatilization model should be more caution to ensure the accurate prediction of ignition characteristics.

Figure 13 illustrates the devolatilization rates before ignition for isolated coal particles with a diameter of 2 mm and T_w of 1123 K under air combustion, when the devolatilization process is described by CPD and TCR model respectively and the ignition criterion is FLC. It can be seen that when devolatilization description changes from TCR to CPD, pyrolysis starts ~0.3 s earlier, which can introduce a noticeable discrepancy in ignition prediction.

For large particles whose intra-particle conduction cannot be ignored, the temperature gradient inside coal particle are more significant. Then, the overall heating rate decreases and thereby the pyrolysis is further postponed when TCR model used, as shown in Fig. 14. Even at the moment of ignition, the overall particle temperature is still lower than that predicted by CPD model.

Figure 15 depicts the τ_i and ignition mode under different X_{O2}'s predicted by the transient ignition model with FLC, while VM is described by CPD and TCR models respectively. It can be seen that as X_{O2} increases, ignition mode is firstly homogeneous, then combined, and finally heterogeneous. In the figure, the inflection point on the τ_i curve indicates the transition of ignition mode caused by the change of X_{O2}. When using TCR, the predicted critical X_{O2} between homogeneous and heterogeneous ignitions increases to 45% from 37% which is predicted by CPD model. This could be attributed to the relatively higher $\tau_{i,homo}$ predicted by TCR.

5. Conclusions

A detailed modeling study of the influences of ignition criteria and devolatilization description on the ignition characteristics of mm-sized isolated coal particles is conducted using a one-dimensional transient ignition model. Some predictions are compared with microgravity experimental data.

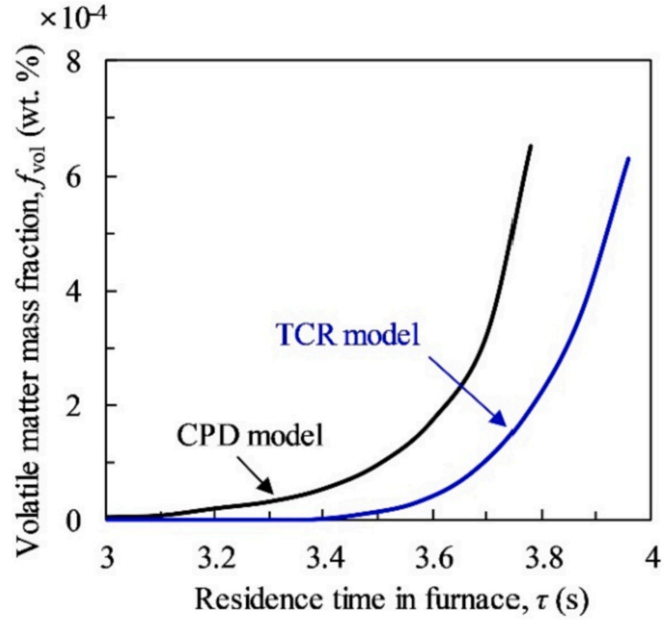

Fig. 13. The comparison of predicted temporal variations of VM mass fraction between CPD and TCR models for isolated coal particles (d_p = 2 mm, T_w = 1123, X_{O2} = 21%).

It is found that the TAC ignition criterion cannot well predict the decreasing trend of T_i with X_{O2}, while FLC ignition criterion fails to well predict T_i when T_w lower than 973 K. The particle center temperature is more reasonable to be used as the characteristic temperature in the ignition prediction.

The combination of devolatilization model and ignition criterium affect the ignition prediction. When devolatilization process is described by CPD model, for homogenous ignition, FLC is more accurate to predict T_i and τ_i than TAC at a higher X_{O2} and a high T_w, while TAC is more accurate to predict τ_i at a large particle size. Using FLC, against TAC, the transient of ignition mode from homogenous to combined happens at a ~80 K higher temperature and ~50 μm larger particle size, while that from combined to heterogenous happens at 250 μm rather than 400 μm. When TCR is used for the devolatilization description, the predicted X_{O2} at which ignition mode changes from homogeneous to heterogeneous is noticeably larger than the one predicted by CPD model.

Two diagrams are respectively given to guide the selection the ignition criterion and identify the ignition mode at a wide range of

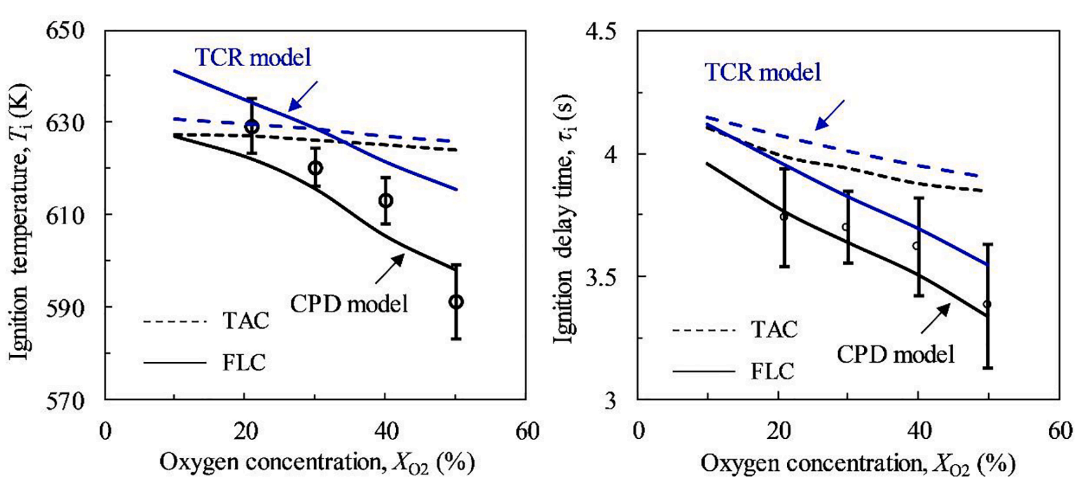

Fig. 12. The predicted variations of T_i and τ_i with X_{O2} for isolated coal particles with different devolatilization model and ignition criteria, with experimental results comparison (d_p = 2 mm, T_w = 1123 K).

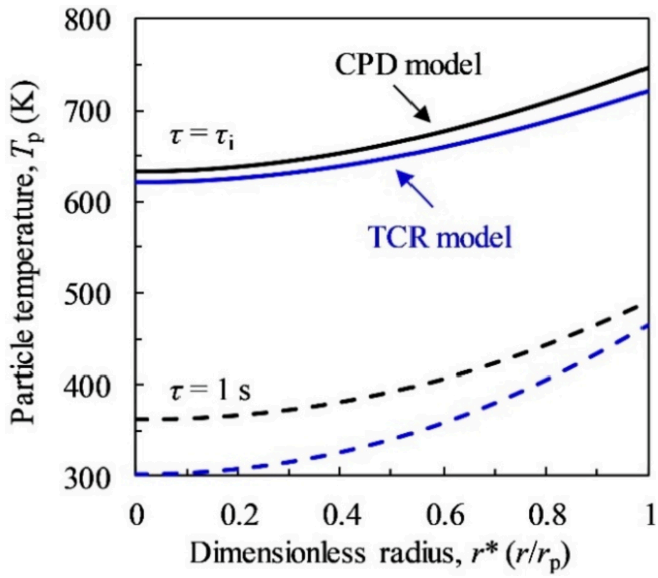

Fig. 14. The comparison of predicated temperature distribution inside coal particles between CPD and TCR models ($d_p = 2$ mm, $T_w = 1123$ K, $X_{O2} = 21\%$).

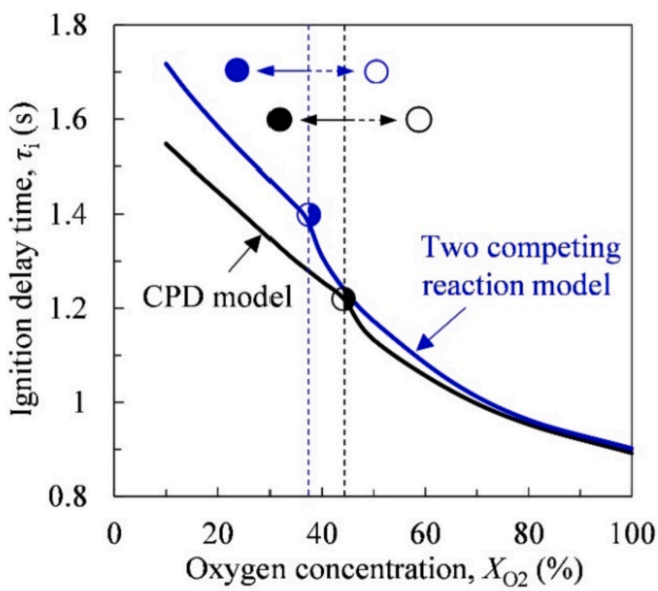

Fig. 15. The comparison of ignition delay time and ignition modes of isolated coal particles under different X_{O2}'s between CPD model and TCR model (Solid point: heterogeneous ignition; Hollow point: homogeneous ignition; Semi-solid point: combined ignition; $d_p = 1$ mm, $T_w = 1123$ K).

conditions.

CRediT authorship contribution statement

Wantao Yang: Conceptualization, Investigation, Writing – original draft. **Yang Zhang:** Validation, Methodology, Writing – review & editing. **Bing Liu:** Investigation, Software, Data curation. **Kailong Xu:** Software, Methodology. **Hai Zhang:** Conceptualization, Supervision.

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.

Acknowledgements

This work was supported by the Natural Science Foundation of China (#11872231 and #U1710251).

References

[1] Annamalai K, Durbetaki P. A theory on transition of ignition phase of coal particles. Combust Flame 1977;29(2):193–208.
[2] Ponzio A, Senthoorselvan S, Yang W, Blasiak W, Eriksson O. Ignition of single coal particles in high-temperature oxidizers with various oxygen concentrations. Fuel 2008;87(6):974–87.
[3] Zhang D-K. Laser-induced ignition of pulverized fuel particles. Combust Flame 1992;90(2):134–42.
[4] Qiao Yu, Zhang L, Binner E, Xu M, Li C-Z. An investigation of the causes of the difference in coal particle ignition temperature between combustion in air and in O_2/CO_2. Fuel 2010;89(11):3381–7.
[5] Essenhigh RH, Misra MK, Shaw DW. Ignition of coal particles: a review. Combust Flame 1989;77(1):3–30.
[6] Yang W, Liu B, Zhang H, Zhang Y, Wu Y, Lyu J. Prediction improvements of ignition characteristics of isolated coal particles with a one-dimensional transient model. Proc Combust Inst 2021;38(3):4083–9.
[7] Du X, Annamalai K. The transient ignition of isolated coal particle. Combust Flame 1994;97(3-4):339–54.
[8] Li S, Xu Y, Gao Q. Measurements and modelling of oxy-fuel coal combustion. Proc Combust Inst 2019;37(3):2643–61.
[9] Zhang M, Yu J, Xu X. A new flame sheet model to reflect the influence of the oxidation of CO on the combustion of a carbon particle. Combust Flame 2005;143(3):150–8.
[10] Yuan Ye, Li S, Li G, Wu N, Yao Q. The transition of heterogeneous–homogeneous ignitions of dispersed coal particle streams. Combust Flame 2014;161(9):2458–68.
[11] Farazi S, Attili A, Kang S, Pitsch H. Numerical study of coal particle ignition in air and oxy-atmosphere. Proc Combust Inst 2019;37(3):2867–74.
[12] Bu C, Gómez-Barea A, Leckner B, Wang X, Zhang J, Piao G. The effect of H_2O on the oxy-fuel combustion of a bituminous coal char particle in a fluidized bed: Experiment and modeling. Combust Flame 2020;218:42–56.
[13] Liu B, Zhang Z, Zhang H, Zhang D. Volatile release and ignition behaviors of single coal particles at different oxygen concentrations under microgravity. Microgravity Sci Technol 2016;28(2):101–8.
[14] Zhu M, Zhang H, Tang G, Liu Q, Lu J, Yue G, et al. Ignition of single coal particle in a hot furnace under normal- and micro-gravity condition. Proc Combust Inst 2009;32(2):2029–35.
[15] Lee H, Choi S. An observation of combustion behavior of a single coal particle entrained into hot gas flow. Combust Flame 2015;162(6):2610–20.
[16] Adeosun A, Xiao Z, Yang Z, Yao Q, Axelbaum RL. The effects of particle size and reducing-to-oxidizing environment on coal stream ignition. Combust Flame 2018;195:282–91.
[17] Zhou K, Lin Q, Hu H, Hu H, Song L. The ignition characteristics and combustion processes of the single coal slime particle under different hot-coflow conditions in N_2/O_2 atmosphere. Energy 2017;136:173–84.
[18] Bu C, Leckner B, Chen X, Pallarès D, Liu D, Gómez-Barea A. Devolatilization of a single fuel particle in a fluidized bed under oxy-combustion conditions. Part A: experimental results. Combust Flame 2015;162(3):797–808.
[19] Wu C, Sun P, Wang X, Huang X, Wang S. Flame extinction of spherical PMMA in microgravity: effect of fuel diameter and conduction. Microgravity Sci Technol 2020;32(6):1065–75.
[20] Zhou K, Lin Q, Hu H, Shan F, Fu W, Zhang P, et al. Ignition and combustion behaviors of single coal slime particles in CO_2/O_2 atmosphere. Combust Flame 2018;194:250–63.
[21] Yang W, Zhang Y, Hu L, Lyu J, Zhang H. An experimental study on ignition of single coal particles at low oxygen concentrations. Front Energy 2021;15(1):38–45.
[22] Richards AP, Fletcher TH. A comparison of simple global kinetic models for coal devolatilization with the CPD model. Fuel 2016;185:171–80.
[23] Fletcher TH, Kerstein AR, Pugmire RJ, Solum MS, Grant DM. Chemical percolation model for devolatilization. 3. Direct use of 13C NMR data to predict effects of coal type. Energ Fuel 1992;6(4):414–31.
[24] Yang G, Tang M, Lu T, Fu W. A study on ignition of large carbon/char particles. J Combust Sci Technol 1995;1(2):162–7.
[25] Katalambula H, Hayashi J-I, Chiba T, Kitano K, Ikeda K. Dependence of single coal particle ignition mechanism on the surrounding volatile matter cloud. Energ Fuel 1997;11(5):1033–9.
[26] Cai R, Zhang H, Zhang M, Yang H, Lyu J, Yue G. Development and application of the design principle of fluidization state specification in CFB coal combustion. Fuel Process Technol 2018;174:41–52.
[27] Feng L, Zhang Q, Wu Y, Huang W, Zhang H. Theoretical analysis on criteria of MILD coal combustion. Energ Fuel 2019;33(11):11923–31.