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Particle Combustion Model Simultaneously Considering a Volatile and Carbon Reaction

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Volatile combustion greatly influences the combustion of solid particles, especially those with a high proportion of volatile content. The processes of volatile releasing and combustion and its effect on particle combustion should be carefully considered to develop an accurate combustion model. A new single particle combustion model considering the volatile effects was established based on the developed "one-film" and "two-film" model, and both radiation and convection effects were considered. Along with the coal combustion, the flame will stay above the particle surface and then move back to the surface; therefore, according to the location of the flame sheet, the gas-phase reaction and surface reaction in the model will change and give the correct calculation. The model focused on the effect of volatiles, and a simulation and comparison have been performed for validation. Additionally, the influence of volatiles, ambient temperature, and particle diameter on the particle combustion has been investigated in this paper. The results show that the new model has sufficient accuracy and a shorter calculation time than other previously reported models and can be used for other complex combustion problems.

1. Introduction

Particle combustion models, including the ignition, combustion, and burnout processes, have been investigated for quite a long time by researchers around the world. Most researchers focused on coal particles, while the combustion of other kinds of particles has not been widely investigated. As for the coal particle ignition, various experimental and theoretical studies have been made to find the mechanisms of ignition.[1−9] The process of coal particle ignition mainly includes three modes: homogeneous ignition, heterogeneous ignition, and joint hetero−homogeneous ignition. Various particle ignition models have been developed according to different modes of ignition, but the difference between the simulation and experimental results has not been satisfactory, especially for homogeneous ignition problems. As for the particle combustion, researchers focus on the burning rate of chars and a series of models for predicting the burning rate of a char particle, including numerical, analytical, and semi-experimental solutions, have been developed.[10−15] The methods used to solve coal particle combustion can be classified into three categories, which are "one-film", "two-film", and continuum models. Some researchers have conducted extensive studies on the continuum model and began to consider the influence of the gas phase and volatile combustion.[16−18] Although the accuracy of the continuum model is much improved, the calculation time has to be shortened to facilitate this model in practical application. Bermudez et al.[19] have worked on the mathematical modeling of the combustion of coal particles in a pulverized coal furnace. A detailed coal particle combustion model was developed in their study considering coal char reactions as well as gas-phase reactions. The approach was instructive, but in nature, the model was a "two-film" coal combustion model. The analysis and comparison of the model have not been carried out in their study; therefore, it is not determined for sure whether the model is accurate or suitable for other complex combustion problems.

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An analysis of previous work showed that most studies were about the coal char combustion. For coal particles with less volatile, it is reasonable to ignore volatile releasing and combustion in the coal char combustion model. However, it would be improper to remove volatile effects when developing a model for other kinds of solid particles, such as wood, biomass, and polymeric materials. Therefore, a new particle combustion model considering volatile effects was established to provide a new solution to simulate the combustion process of different kinds of particles for practical application.

2. Numerical Model

A coal particle was adopted to build the combustion model to make the validation much easier. The assumptions when establishing the model include the following: (1) The coal particle only consists of two parts, char and volatiles, and ignores the change of the porosity of the coal particle when pyrolzing and burning. (2) The coal particle is supposed to be spherical and burning in a quiescent, infinite, ambient medium that contains only oxygen and an inert gas, such as nitrogen. (3) The flame is supposed to be unlimited thin, and spherically symmetric around the coal particle. (4) The pyrolyzing and burning process is quasi-steady. (5) All of the volatile matter is regarded as CH_4.[7,17,18] Similarly, "one-film" and "two-film" models were adopted in different conditions to describe the whole combustion process. The classical "one-film" model assumes that only oxidation of coal char occurs at the particle surface producing CO and/or CO_2,[20,21] including two reactions: $C + 1/2O_2 \rightarrow CO$ and $C + O_2 \rightarrow CO_2$. The "one-film" model adopted in this paper was extended and supposed that, when the flame was on the particle surface, the oxidation of coal char and volatile matter happened on the surface with CO_2 and H_2O as the main products. The classical "two-film" model assumes that a deoxidization reaction, $C + CO_2 \rightarrow 2CO$, occurs on the particle surface and a volumetric reaction, $CO + 1/2O_2 \rightarrow CO_2$, happens at the flame sheet.[20,21] Therefore, when the flame was off of the particle surface, the volatile matter CH_4 and the product of surface oxidation were supposed to burn at the flame sheet. The gas-phase reaction was assumed to be infinitely fast. (6) The physical properties of coal and gas, such as the gas-phase thermal conductivity, specific heat, and particle density, are all constant at a certain surface temperature. Furthermore, the Lewis number is assumed to be unite, i.e., Le = 1. (7) The particle is of uniform temperature and radiates as a gray body to the surroundings without participation of the intervening medium.

2.1. Pyrolyzing Model. On the basis of the assumption above, the coal particle contains the fixed carbon and volatiles. The pyrolysis process is subjected to the volatiles and not affected by the fixed carbon. In addition, the particle density stays the same, but the particle diameter will change during the pyrolysis process. The "two-step" devolatilization model was introduced to describe the pyrolysis process

$$m_0 = m_{v0} + m_{c0} \tag{1}$$

$$m_v = m_{v0} \exp\left(-\int_0^t (k_1 + k_2) dt\right) \tag{2}$$

$$\dot{m}_g = m_v(\alpha_1 k_1 + \alpha_2 k_2) \tag{3}$$

$$k_1 = A_1 \exp(-E_1/(R_u T_s)) \tag{4}$$

$$k_2 = A_2 \exp(-E_2/(R_u T_s)) \tag{5}$$

where m_0, m_{v0}, and m_{c0} are the initial quantity of the coal particle, volatile, and fixed carbon (kg), respectively, m_v is the quantity of volatile at t moment (kg), $\dot{m}_g$ is the volatile releasing

from the particle (kg/s), k_1 and k_2 are the rate coefficients of pyrolysis (s^{-1}), α_1 and α_2 are the stoichiometric coefficients with values of 0.38 and 0.8, respectively, E_1 and E_2 are the pyrolysis activation energies (J/mol), A_1 and A_2 are the pre-exponential factors (s^{-1}), R_u is the universal gas constant with a value of 8.3145 J mol^{-1} K^{-1}, and T_s is the surface temperature (K).

2.2. Combustion Model with Flame on the Surface. When the flame sheet is on the particle surface, the main products are CO_2 and H_2O and the main reactions on the surface are

$$C + vsO_2 = (1 + vs)CO_2 \tag{a}$$

$$CH_4 + f_1 O_2 = f_2 CO_2 + f_3 H_2O \tag{b}$$
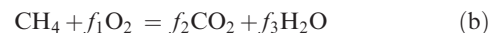
where vs, f_1, f_2, and f_3 are the stoichiometric coefficients. Between the particle and surroundings, i.e., $r_s \rightarrow \infty$, the oxygen diffusion equation by Fick's law can be simplified to

$$\dot{m}_c = \frac{4\pi r \rho_s D}{vs + Y_{O_2}} \frac{dY_{O_2}}{dr} - \frac{f_1 + Y_{O_2}}{vs + Y_{O_2}} \dot{m}_g \tag{6}$$

The boundary conditions that apply to the equation are $r = r_s$, $Y_{O_2} = Y_{O_2,s}$, and $r \rightarrow \infty$, $Y_{O_2} = Y_{O_2,\infty}$

According to ref 22, the surface reaction is assumed to be first-order with respect to O_2 and the carbon reaction rate can be expressed as

$$\dot{m}_c = 4\pi r_s^2 k_c \frac{W_C W_{mix}}{W_{O_2}} \frac{p}{R_u T_s} Y_{O_2,s} \tag{7}$$

$$k_c = A_3 \exp(-E_3/(R_u T_s)) \tag{8}$$

where $\dot{m}_c$ is the fixed carbon reaction rate (kg/s), ρ_s is the particle density (kg/m^3), D is the diffusion coefficient (m^2/s), $Y_{O_2,s}$ and $Y_{O_2,\infty}$ are the mass fraction of O_2 on the surface and in the ambient, r_s is the particle radius (m), W_C, W_{mix}, and W_{O_2} are the molecular weight of C, gas phase, and O_2 (g/mol), respectively, p is the ambient pressure (Pa), k_c and A_3 are the rate coefficient and pre-exponential factor of reaction a (m/s), respectively, and E_3 is the activation energy of reaction a (J/mol).

When the surface temperature is defined, the reaction rate of volatile and fixed carbon can be obtained by solving the equations above. Unfortunately, in most cases, the surface temperature is unknown and the energy equation is needed to solve the surface temperature and simulate the combustion process

$$c_s m \frac{dT_s}{dt} = \dot{m}_c \Delta h_3 + \dot{m}_g \Delta h_2 - \dot{Q}_{conv} - \dot{Q}_{rad} - \dot{m}_g q - \dot{m}_c (c_s - c_p) T_s \tag{9}$$

$$m = \frac{4}{3} \pi r_s^3 \rho_s \tag{10}$$

$$\dot{Q}_{conv} = \frac{\lambda_s}{2r_s} (T_s - T_\infty) \tag{11}$$

$$\dot{Q}_{rad} = 4\pi r_s^2 \varepsilon \sigma (T_s^4 - T_\infty^4) \tag{12}$$

where m is the particle quality (kg), c_s and c_p are the specific heats of the particle and gas (J kg^{-1} K^{-1}), respectively, Δh_3 and Δh_2 are the heat of reactions a and b (J/kg), $\dot{Q}_{conv}$ is the convective heat (J/kg), $\dot{Q}_{rad}$ is the radiation energy (J/kg), q is the heat of the pyrolysis reaction absorbed with a value of 8.37×10^5 J/kg, λ_s is the gas-phase thermal conductivity (W m^{-1} K^{-1}), T_∞ is the ambient temperature (K), ε is the emissivity of the particle surface with the value of 0.8, and σ is the Stefan−Boltzmann constant with the value of 5.67×10^{-8} W m^{-2} K^{-4}.

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With the development of the burning process, the flame sheet will be off from the particle surface and it would be improper to describe the combustion process by the model above. Another model with the same pyrolysis model should be developed.

2.3. Combustion Model with Flame off of the Surface. A chemical reaction will happen simultaneously on the particle surface and the flame sheet as the flame is not on the surface. The dominant surface and gas-phase reactions are

$$C + vs_1CO_2 = (1 + vs_1)CO \tag{c}$$

$$2CO + O_2 = 2CO_2 \tag{d}$$

$$CH_4 + f_1O_2 = f_2CO_2 + f_3H_2O$$
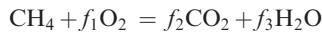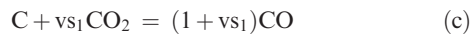
where vs_1 is the stoichiometric coefficient of reaction c.

Similarly, according to Fick's law, the diffusion equations of each gas will be established in the field $r_s \rightarrow r_f$ and $r_f \rightarrow \infty$.

(1) $r_s \rightarrow r_f$, the conservation of CO_2 is expressed as

$$\dot{m}_c = \frac{4\pi r^2 \rho_s D}{1 + Y_{CO_2}/vs_1} \frac{d(Y_{CO_2}/vs_1)}{dr} - \frac{Y_{CO_2}/vs_1}{1 + Y_{CO_2}/vs_1} \dot{m}_g \tag{13}$$

with boundary conditions: $r = r_s$, $Y_{CO_2} = Y_{CO_2,s}$, and $r = r_f$, $Y_{CO_2} = Y_{CO_2,f}$.

(2) $r_f \rightarrow \infty$, the diffusion equation of CO_2 can be simplified as

$$\dot{m}_c = \frac{4\pi r^2 \rho_s D}{Y_{CO_2}/vs_1 - 1} \frac{d(Y_{CO_2}/vs_1)}{dr} + \frac{f_2/vs_1 - Y_{CO_2}/vs_1}{Y_{CO_2}/vs_1 - 1} \dot{m}_g \tag{14}$$

with boundary conditions: $r = r_f$, $Y_{CO_2} = Y_{CO_2,f}$, and $r \rightarrow \infty$, $Y_{CO_2} = 0$.

(3) $r_f \rightarrow \infty$, the conservation of the inert gas can be expressed as

$$\dot{m}_c = \frac{4\pi r^2 \rho_s D}{Y_{N_2}} \frac{d(Y_{N_2})}{dr} - \dot{m}_g \tag{15}$$

with boundary conditions: $r = r_f$, $Y_{N_2} = Y_{N_2,f}$, and $r \rightarrow \infty$, $Y_{N_2} = Y_{N_2,\infty}$.

(4) $r_f \rightarrow \infty$, the diffusion equation of H_2O can be described as

$$\dot{m}_c = \frac{4\pi r^2 \rho_s D}{Y_{H_2O}} \frac{d(Y_{H_2O})}{dr} + \frac{f_3 - Y_{H_2O}}{Y_{H_2O}} \dot{m}_g \tag{16}$$

with boundary conditions: $r = r_f$, $Y_{H_2O} = Y_{H_2O,f}$, and $r \rightarrow \infty$, $Y_{H_2O} = 0$.

Furthermore, from $\sum Y_i = 1$ and completely consumed of O_2 at the flame sheet, the following equation is added:

$$Y_{CO_2,f} + Y_{H_2O} + Y_{N_2,f} = 1 \tag{17}$$

Equations 13−17 can be manipulated to eliminate all of the variables, except $\dot{m}_c$ and $Y_{CO_2,s}$

$$Y_{CO_2,s} = [(-b_2(ab_2Y_{O_2,\infty} + b_1b_2vs_1 + b_1b_3 - ab_1Y_{N_2,\infty}))/$$
$$(ab_2 - b_2b_2vs_1 - b_2b_3)\exp(-a/r_s) - b_1]a/r_s \tag{18}$$

$$a = (\dot{m}_c + \dot{m}_g)/(4\pi\rho_s D) \tag{19}$$

$$b_1 = \dot{m}_c/(4\pi\rho_s D) \tag{20}$$

$$b_2 = \left(\dot{m}_c + \frac{f_2}{vs_1}\dot{m}_g\right)/(4\pi\rho_s D) \tag{21}$$

$$b_3 = f_3\dot{m}_g/(4\pi\rho_s D) \tag{22}$$

where $Y_{CO_2,s}$ and $Y_{CO_2,f}$ are the mass fractions of CO_2 on the surface and flame sheet, respectively, $Y_{N_2,f}$ and $Y_{N_2,\infty}$ are the mass fractions of N_2 on the flame and in the surroundings,

respectively, $Y_{H_2O,f}$ is the mass fraction of vaporized water on the flame, and r_f is the flame radius (m). Similarly, the surface reaction is also assumed to be first-order in the CO_2 concentration; thus, the rate is expressed as

$$\dot{m}_c = 4\pi r_s^2 k_{c1} \frac{W_C W_{mix}}{W_{CO_2}} \frac{p}{R_u T_s} Y_{CO_2,s} \tag{23}$$

$$k_{c1} = A_4 \exp(-E_4/(R_u T_s)) \tag{24}$$

where W_{CO_2} is the molecular weight of CO_2 (g/mol), k_{c1} and A_4 are the rate coefficient and pre-exponential factor of reaction c (m/s), respectively, and E_4 is the activation energy of reaction c (J/mol).

Similarly, to obtain the surface temperature, it is necessary to solve the energy balance on the surface and the flame sheet

$$c_s m \frac{dT_s}{dt} = \dot{m}_c \Delta h + \dot{Q}_{conv1} - \dot{Q}_{rad} - \dot{m}_g q - \dot{m}_c(c_s - c_p)T_s \tag{25}$$

$$\dot{m}_c\Delta h_1 + \dot{m}_g\Delta h_2 - 4\pi r_f^2 \varepsilon\sigma(T_f^4 - T_\infty^4)$$
$$= c_p[((T_s - T_f)\exp(-Z_t\dot{m}_c/r_f))/(\exp(-Z_t\dot{m}_c/r_s)$$
$$- \exp(-Z_t\dot{m}_c/r_f))$$
$$- (\dot{m}_c(T_\infty - T_f)\exp(-Z_t\dot{m}_c/r_f))/(1 - \exp(-Z_t\dot{m}_c/r_f))] \tag{26}$$

$$\dot{Q}_{conv1} = \frac{\lambda_s}{2r_s}(T_s - T_f) \tag{27}$$

$$Z_t = \frac{c_p}{4\pi\lambda_s} \tag{28}$$

where $\dot{Q}_{conv1}$ is the convective heat between the particle and flame (J/kg), Δh and Δh_1 are the released heat of reactions c and d (J/kg), respectively, and T_f is the flame temperature (K).

According to the assumption above, the particle density was supposed to be constant in the combustion process. To describe the whole combustion process, the mass conservation equation should be added to complete the model.

$$\frac{dr_s}{dt} = -\frac{\dot{m}_c + \dot{m}_g}{4\pi r_s^2 \rho_s} \tag{29}$$

Equations 1−29 are then solved simultaneously to describe the whole process of volatile releasing and combustion, carbon combustion, and particle burnout. When simulating a particle combustion process, eqs 1−5 will be executed to determine the releasing rate of CH_4. When the flame radius is smaller than or equal to the particle radius, eqs 6−12 will be used to determine the variation of the particle temperature and combustion rate. When the flame is off of the particle surface, eqs 13−29 will give the correct calculation of the combustion rate. The boundary conditions were that the coal particle was supposed to be in a quiescent and high-temperature atmosphere with only O_2 and N_2 and the particle combustion happened under normal gravity conditions with radiation and convection effects considered.

3. Results and Discussion

Simulations of coal particle combustion have been arranged by the model developed above, and the results are compared to studies and experiments reported previously. A brief discussion and analysis of the results has also been carried out. A coal particle with a diameter of 80 μm was used to validate the model and analyze the influence of different factors on the combustion process. The parameters of the pyrolysis reaction and combustion reactions are shown in Table 1.[13,31] However, when the new model developed was
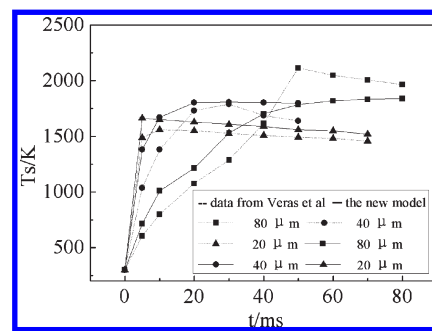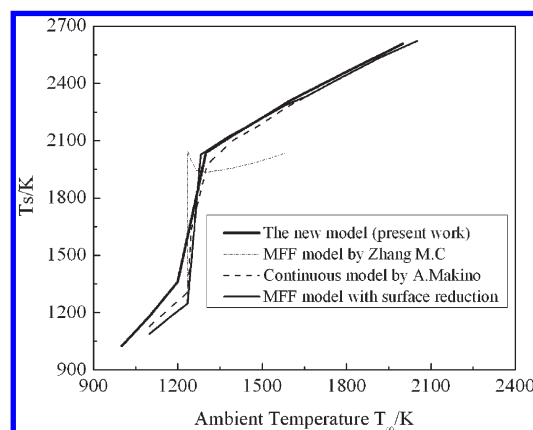
Table 1. Particle Properties and Reaction Parameters

particle properties	diameter (μm)		density (kg/m^3)		volatile fraction (%)	
	80		1350		43.8	
	pre-exponential factor (s^{-1})		activation energy (J/mol)		stoichiometric coefficient	
parameter of pyrolysis reaction	A_1	A_2	E_1	E_2	α_1	α_2
	3.7×10^5	1.46×10^{13}	7.4×10^4	2.5×10^5	0.38	0.8
parameter of combustion	pre-exponential factor (m/s)		activation energy (J/mol)		reaction heat (J/kg)	
$C + O_2 \rightarrow CO_2$	1.2×10^4		1.01×10^5		3.289×10^7	
$C + CO_2 \rightarrow CO$	6.2×10^7		2.7×10^5		-14.23×10^6	
$CO + O_2 \rightarrow CO_2$					10.11×10^6	
$CH_4 + O_2 \rightarrow CO_2 + H_2O$					5.025×10^7	
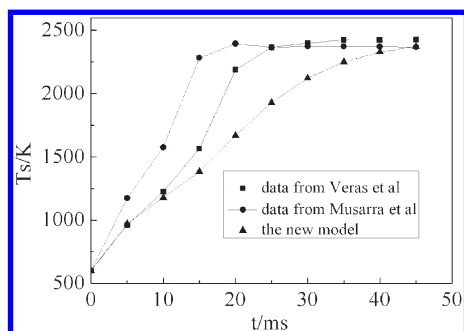
Figure 1. Comparison of calculated particle temperature to the modeling predictions by Veras et al.[23] and Musarra et al.[24]

Figure 2. Comparison of the calculated particle temperature to the modeling predictions of Veras et al.[23] at different particle diameters.

Figure 3. Comparison of the new model developed with other models.

compared to different coal particles at different conditions, the kinetic parameter and those used for the reaction may be very different from each other. The paper adjusted some parameters to keep them the same as those used in the references published previously.

3.1. Comparison. The initial particle temperature is supposed to be 600 K; the ambient temperature is 1800 K; and the mass fraction of O_2 is supposed to be 0.233. The comparison of results between this work and data reported previously[23,24] is shown in Figure 1. The results demonstrate that the calculated data from the model developed in this paper is in a reasonable agreement with data from the references. The difference may be attributed to three reasons. First, the model reported previously did not consider the heat absorbed in the process of pyrolysis; therefore, the particle temperature increased much more quickly. Second, the model in the reference considered another surface reaction, $C + O_2 \rightarrow CO$, which has a much higher reaction rate at high temperatures, and this will also increase the particle temperature. Removal of this reaction in this paper was based on two reasons. The first one was that the new model developed in this study was actually a combination of the "one-film" and "two-film" models. When the coal particle has been ignited for a while, the particle temperature was quite high and the "one-film" model, which was proven to be quite accurate in this situation, was governing the combustion process. Therefore, the total accuracy would not be affected. The second one was that removal of this reaction made the model simpler and calculation time much less. Finally, not all of the reaction parameters were given in the

references; thus, there may be a difference between the reaction parameters used in this work and those in the references.

Figure 2 shows the surface temperature of particles with different diameters under the conditions of ambient temperature of 1400 K and initial particle temperature of 300 K. The comparison of results can further prove the accuracy of the developed model in this study. Figure 3 shows the comparison between the results in the present work and the results reported previously.[25] The initial diameter of the coal particle is 50 μm, with a constant O_2 partial pressure of 0.01 MPa. All of the kinetic parameters were defined and chosen the same as those in ref [25], and those for reactions c and d

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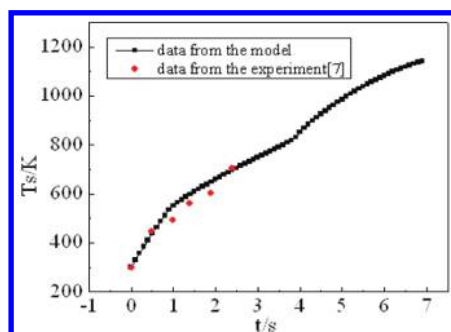(25) Zhang, M. C.; Yu, J.; Xu, X. C. *Combust. Flame* **2005**, *143*, 150–158.

Figure 4. Comparison of the calculated particle temperature to the experimental data of Zhu et al.[7]

were taken from Howard et al.[26] and Essenhigh,[27] respectively. It can be seen that reasonable agreement was achieved between the new model and the continuous film model developed by Makino and Law[13,16] and the MFF model developed by Zhang et al.[17,18,20,21] in predicting the ignition of coal particles. Figure 4 shows the variation of the particle temperature predicted against the experimental data,[7] with the ambient temperature of 1123 K, initial particle temperature of 300 K, and initial particle diameter of 2.0 mm. It can be seen that the simulation data agreed well with the experimental data. The ignition temperature predicted by the new model is about 800 K, which is different from the ignition temperature of 710 K in the experiment. However, according to ref 7, it concluded that the ignition temperature was almost 50−80 K lower in microgravity conditions than in normal gravity conditions; therefore, it means that the model developed can predict the ignition temperature correctly, the assumption used to develop the model was reasonable, and the model was accurate enough to describe the particle combustion. Furthermore, in comparison to the continuum model that is the most accurate, the calculation time of the new model is several times shorter under the same case. The model is quite suitable for practical application.

3.2. Influence of Volatiles on Particle Combustion. The combustion of most fuels mainly starts at the reaction of volatiles; therefore, it is very important to consider the influence of volatiles in the combustion model to predict the ignition process. In fire research, it can be found that almost all of the fires are caused by wood and polymeric materials, such as polyvinyl chloride (PVC) burning. The fraction of volatiles in these kinds of materials is quite high, and the combustion process is very rapid and intensive. Therefore, the combustion model of these materials should carefully take the volatile effect into account. On the basis of the combustion model established above, the influence of volatiles on particle burning was briefly investigated.

Figure 5 shows the relations between the volatile burning and particle ignition under the conditions that the ambient temperature is 1000 K and the particle diameter is 80 μm. When the particle is only char and no volatile, the surface temperature increases and then does not change when an energy balance is satisfied between the particle and the surroundings. Ignition did not happen in this situation. When the coal particle contains a certain proportion of volatiles, with the temperature increasing, the volatile releasing rate increased

significantly and ignited. At $t = 50$ ms, after the volatile flame quenched, the temperature of the carbon particle was quite high and ignition happened then to further increase the particle temperature. The mode of ignition is just the joint hetero−homogeneous ignition discovered and defined by Jüntgen et al.[28]

3.3. Influence of the Ambient Temperature on Particle Combustion. Figure 6 presents the predicted surface temperature and diameter change of a 80 μm coal particle under different ambient temperatures. Figure 6a shows that, with ambient temperature increasing, the ignition happened earlier but the influence of volatile combustion on particle ignition became less. In addition, the pyrolysis and surface chemical reaction rate accelerated and the particle diameter decreased with an increasing ambient temperature. As shown in Figure 6b, the change of the particle diameter can be divided into two phases. The first rapid decrease phase happened between 10 and 50 ms, which was caused by sudden acceleration of the pyrolysis process. The second phase occurred after the volatiles were completely consumed, and the change of diameter was mainly attributed to carbon combustion. Furthermore, it can be seen from Figure 6b that the flame location changed with time. When the particle was ignited, the flame propagated far away from the surface and developed its maximum value when the pyrolysis rate reached its maximum. Along with the combustion, the flame then returned back to the surface.

3.4. Influence of Diameters on Particle Combustion. Figure 7 gives the variation of the surface temperature and the combustion rate of particles with different diameters (particle diameters of 20, 40, and 80 μm) when the ambient temperature is 950, 1000, and 1300 K, respectively. According to the conclusions in ref 29, when the particle diameter is less than 6 mm, there will be a sudden increase of the temperature in the combustion process. When the equation $d^2T_s/dt^2 = 0$ is satisfied, it indicates that the particle has been ignited. Therefore, in this study, this equation was used as the criteria of ignition. As shown in panels a and b of Figure 7, smaller particles need a higher ambient temperature to ignite and maintain the combustion. Especially, in Figure 7b, when the particle diameter increases from 20 to 100 μm, the ignition temperature decreases from almost 1300 to 950 K, which demonstrates that the ignition temperature of smaller particles is a little higher. The reason is that the heat loss per unit area of small particles is higher and only a much higher ambient temperature can supply enough energy to ignite them. This phenomenon is in coincidence with the conclusion of ref 30. Figure 7c shows the relationships between the combustion rate per unit area and particle diameter during the period after ignition. The results demonstrate that the combustion rate per unit area of a small particle is higher than that of a bigger particle; therefore, the temperature of a small particle is higher during the combustion process.

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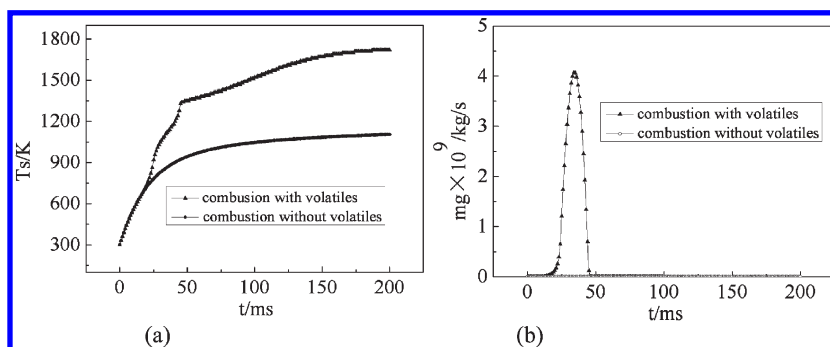
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Figure 5. Influence of volatile combustion on coal combustion: (a) influence on the particle surface temperature and (b) influence on the volatile releasing rate.
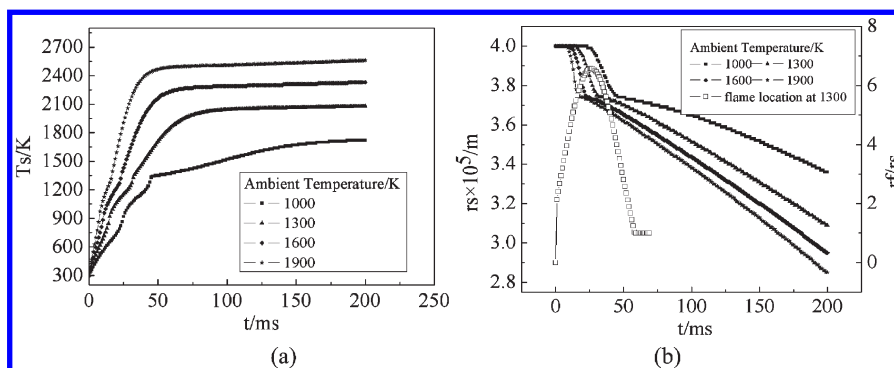

Figure 6. Influence of the ambient temperature on coal combustion: (a) influence on the particle surface temperature and (b) influence on the particle radius.
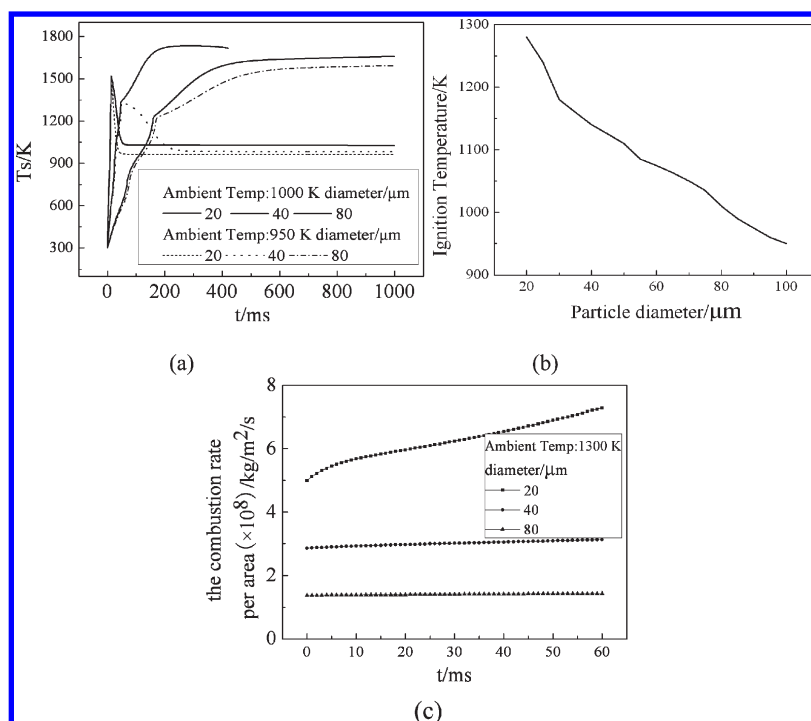

Figure 7. Influence of the particle diameter on coal combustion: (a) influence on the particle surface temperature, (b) influence on the ignition temperature, and (c) influence on the combustion rate per unit area.

4. Conclusions

To develop a particle combustion model for practical application and extend the coal particle model to other particles, such as high volatile fuels, a new combustion model considering volatile effects was developed by integrating "one-film" and "two-film" models. The new model simultaneously considered the volatile releasing and burning and the fixed carbon reacting and burning. In the particle combustion, the flame of the particle will change its location during the burning process. Therefore, judging from the location of the

flame sheet, the gas-phase reaction and surface reaction in the model will change and give the correct calculation. In addition, some numerical simulations have been carried out, and the results of the new model have been compared to other studies and experiments previously reported. The results demonstrated that the new model has adequate accuracy and quite a shorter calculation time. Furthermore, on the basis of the new model, the influence of several factors on the particle combustion has been investigated, some instructive conclusions have been obtained and agreed well with results and conclusions from other researchers, and the accuracy of the new model was proven again.

However, the model developed still has some aspects to be further improved. The accuracy of the new model can be further improved by considering the surface reaction in more detail and increasing the components of volatile matter.