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Effects of particle sizes on transport phenomena in single char combustion

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Abstract

A one-dimensional char combustion model including pore structure effects is used to numerically investigate single char particle combustion for several different types of char samples. Previously, it is expected that small char particles have less combustion time. However, the present work shows that this is true only if the combustion time is defined as that needed for a char particle diameter diminished below a certain value. If the combustion time is defined as time needed for the carbon conversion ratio higher than a certain value, there are optimal particle sizes in a limited combustion period. Just reducing the char particle sizes may not get high carbon conversion ratios. It has also been found that, in general, the larger particles have higher temperatures at the exterior surfaces.

Keywords: Mass transfer; Porous media; Char combustion; Fractal

1. Introduction

Char combustion is very important for both pulverized coal boilers and fluidized bed boilers. It is well known that char particle sizes significantly affect char combustion. The heat transfer coefficient at the particle surface and the oxygen diffusion from the bulk flow to the particle surface are usually dependent on the particle diameters. For coal combustion, it is believed that, when coal particle diameters are under 100 microns, the char reaction is chemically controlled [1]. For coal particles above 100 microns, the burning time is proportional to the square of the diameter, and for coal particles under 100 microns, proportional to the 0.4 power of the diameter [1–3]. The particle size effects are different for high environmental temperature and relative low environmental temperature. At high temperature, the combustion of small char particles is mainly under the chemical control and may partly be affected by the diffusion control, as in pulverized coal combustion boilers. In fluidized beds, the environmental temperature is relatively low and the particle size is relatively large. The char combustion is under diffusion control for these large particles.

In char combustion, the particle sizes also affect mass transfer, heat transfer, combustion rates, and so on [4,5]. Generally, the smaller a char particle size is, the faster the char combustion is. However, it is difficult to investigate the effects of single char particle size on char combustion if the char particle size is small. The expectation that a smaller char particle burns faster actually is not supported by solid experimental data.

This paper numerically investigates single char particle combustion with a one-dimensional model. The model includes the effects of pore structures in combustion combined with heat and mass transfer. It is believed that char pore structures play an important role in char combustion. Char particles are burned at the exterior and interior surface areas in most time. Firstly, oxygen diffuses from the bulk flow to the exterior surface

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Nomenclature

$C_{O_2}^{(s)}$	oxygen concentration at char surface (mol/m^3)
$C_p^{(c)}$	specific heat capacity of the char particle
D	pseudo-binary diffusion coefficient for O_2 and CO_2 (m^2/s)
d_i	arithmetic mean diameter of the ith group particles
d_m	mean diameter with respect to the mass
G	char combustion rate (kg m^{-2}s^{-1})
H	heat released from the carbon combustion ($=94$ kcal/mol)
h	convection heat transfer coefficient
k	char chemical reaction rate in Arrhenius form
m	mass of the particle
N_i	particle number for the ith group
N	total particle number
P	total pressure (Pa)
Q	carbon reaction rate (mol/s)
R	ideal gas constant [$=8.314$ J/(mol K)]
r_s	radius of the char particle (m)
S	total reaction surface areas (m^2)
s_l	specific macro-pore surface areas (m^2/kg)
T_m	gas mean temperature for $r_s < r < r_\infty$ (K)
T_p	temperature at the particle surface (K)
T_w	wall temperature (K)
T_∞	temperature of the surrounding bulk flow (K)
$y_{O_2}^{(b)}$	oxygen mole fraction at the bulk flow
$y_{O_2}^{(s)}$	oxygen mole fraction at the char particle surface
ρ	char density (kg/m^3)
η	initial ash content ratio
β	fractal geometrical factor
ε	emissivity (taken as 0.7)
σ	Boltzman constant
λ_g	surrounding gas thermal conductivity

of char particles. The reacted gas products also diffuse from the particle exterior surface to the bulk flow. Oxygen will also diffuse into char pores and reacted at the interior surface. The reacted gas products in the pores also diffuse to outside of the pores. All these gas diffusions affect char combustion. Because different chars have different pore structures, the rates of gas diffusions in the pores are different. Therefore, chars from different parent coals have different apparent combust rates.

The geometrical shapes of char pores are very complex and it is difficult to describe their effects on char combustion by traditional methods. However, it has been found that char pores have fractal-like structures. The properties of gas diffusion within fractal pore media are different from that described by Fick's diffusion law. He et al. [6] has presented a fractal geometrical index and the relations of this index and combustion rates have been investigated. In this paper, size effects on char combustion is to be analyzed for several different types of char samples. A char combustion model including pore structure effects is combined with a simple mass transfer model for single char particle combustion.

2. Mathematical model

In general, there are several processes in single char combustion. Firstly, the oxygen diffuses toward the char particle surface and continues to diffuse into char pores. Combustion can occur both at the exterior surface and interior surface. After combustion, the reacted products will diffuse from the pores and the exterior surface to the bulk flow.

2.1. Mass transfer around char particle

Consider a char particle with an initial room temperature injected into a high temperature bulk flow. The mass transfer rate of oxygen from the bulk flow to the particle surface depends on the chemical reaction of char. There are many possibilities of carbon reactions at the particle surface. For the purpose of the simplification, the following three are most common mentioned in literature:

$$C + O_2 \rightarrow CO_2 - (H : 94\ \text{kcal/mol}) \tag{1}$$

$$C + \tfrac{1}{2}O_2 \rightarrow CO \tag{2}$$

$$C + CO_2 \rightarrow 2CO \tag{3}$$

The apparent reaction order varies from 0 to 1 under experimental conditions [1,4,5,7,8]. In this paper, it is assumed that the apparent reaction order is 1 and the char chemical reaction is expressed in the form of Eq. (1).

Suppose that the carbon particle has sphere shape and the relative speed of the char particle and its surrounding air is very small. This is true in both pulverized coal boilers and fluidized beds for small char particles. Therefore, the char particle can be assumed to be burned in stagnant air. The mass transfer process near the particle sphere can be illustrated in Fig. 1. At time, t, Q (mol/s) carbon is reacted. According to Eq. (1), the reacted O_2 is Q (mol/s) and the released CO_2 is Q (mol/s). Then, the inward oxygen is Q (mol/s) and the outward CO_2 is Q (mol/s). The consumed oxygen (and the reacted carbon) Q at the atmosphere pressure can be calculated as [9]

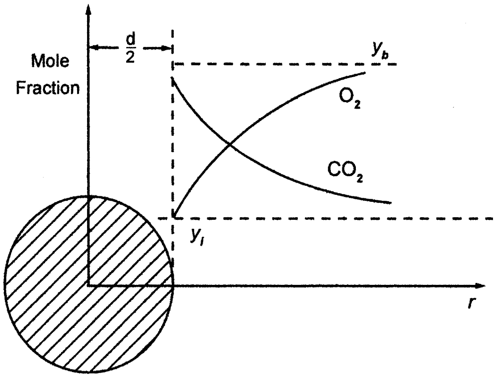

Fig. 1. Illustration of mass transfer around single char particle.

$$Q = \frac{4 \times 10^5 \pi r_s D}{RT_m}(y_{O_2}^{(b)} - y_{O_2}^{(s)}) \tag{4}$$

T_p represents the temperature at the particle surface and T_∞ the temperature of the surrounding bulk flow. Therefore, the mean temperature is determined as

$$T_m = \frac{T_p + T_\infty}{2} \tag{5}$$

The pseudo-binary diffusion coefficient is the function of the particle temperature and can be written as [10]

$$D = 0.138\left(\frac{T}{273}\right)^{1.80} \quad (\text{cm}^2/\text{s}) \tag{6}$$

2.2. Char combustion

Char combustion rate can be expressed as

$$Q = SkC_{O_2}^{(s)} \tag{7}$$

where k is the reaction rate expressed in Arrhenius form as

$$k = A_1 \exp\left(-\frac{E_1}{RT_p}\right) \tag{8}$$

For a porous sphere particle, the total reaction surface includes the exterior surface and internal surface in pores. In char combustion modeling, one of the most difficult problems is to determine char burning within pores. The char combustion rate should relate to the gas diffusions within pores. There are two factors should be considered during char pore surface burning: (1) the pore reaction surface area; (2) the oxygen concentration at the pore reaction surface. Oxygen may not penetrate to the core center of the particle during combustion and not all the pore surface area is the pore reaction surface. For the pore reaction surface of the particles, the oxygen concentration is also different from one site to another site.

In this paper, the char combustion model presented by He et al. [6] is used. In this model, the char pores are classified as macro-pores and micro-pores. The macro-pores are considered mainly as the pore reaction surface area. Then, the reaction surface for the char sphere illustrated in Fig. 1 can be approximately considered as the macro-pore surface and particle exterior surface:

$$S = \left(4\pi r_s^2 + \frac{4}{3}\rho s_l \pi r_s^3\right) \tag{9}$$

The specific macro-pore surface area (m^2/kg), s_l, is defined in [6,11]. In general, char particles contain a certain amount of ash. It is assumed that the ash distributes uniformly in the char particle and the carbon reaction surface area is the char reaction surface area removing ash surface area. Then,

$$S = \left(4\pi r_s^2 + \frac{4}{3}\rho s_l \pi r_s^3\right)(1 - \eta) \tag{10}$$

where η are the initial ash contents (%).

The O_2 concentration at char surface is expressed as

$$C_{O_2}^{(s)} = \frac{10^5 y_{O_2}^{(s)}}{RT_p} \tag{11}$$

The effects of different oxygen concentration at different pore reaction surface sites are implicitly included in Arrhenius expression. Actually, the "average effects" of oxygen concentration, as well as gas diffusion effects, at pore reaction surface are included in the apparent activation energy and pre-exponential factor. Then, the reaction rate is

$$k = 0.14\exp(16\beta)\exp\left(-\frac{150 \times 10^3 \beta}{RT_p}\right) \times \exp\left(-\frac{54 \times 10^3}{RT_p}\right) \tag{12}$$

Therefore, the reaction rate is

$$Q = 0.14 \times 10^5 \left(4\pi r_s^2 + \frac{4}{3}\rho s_l \pi r_s^3\right)(1 - \eta)\frac{y_{O_2}^{(s)}}{RT_p} \times \exp(16\beta)\exp\left(-\frac{150 \times 10^3 \beta}{RT_p}\right) \times \exp\left(-\frac{54 \times 10^3}{RT_p}\right) \tag{13}$$

where β is the fractal geometrical factor [6] deduced from the experimental data. Different chars have different pore parameters.

During char combustion, the particles burn with reduction in size but at a constant density, or burn with reduction in density at a constant size. There is also a case that the particles burn with reduction in both size and density [4,12,13]. In this paper, as done by many other researchers, it is assumed that the particles are burned with reduction in size at constant density.

During coal gasification and char combustion the specific pore surface area measured by a BET is usually changed [14,15]. However, during char combustion at high heating rate, statistically, the specific pore surface area of char measured by a mercury porosimetry is approximately unchanged [11]. Comparing with pores measured by a BET, the pore sizes measured by the mercury porosimetry are much larger. In this paper, the surface area of the macro-pores is important for char combustion [6,11], and furthermore, during char combustion, the fractal dimensions and the ratios of the macro-pore surface to the total pore surface are unchanged [11]. Therefore, the parameter β and the specific reaction surface are constant during different char conversion periods.

Although the apparent activation energy and pre-exponential factor in Eq. (8) can also be deduced directly from the experimental data [16], Eq. (12) is preferred for the expression of the reaction rate, k, due to the following reason: Eq. (12) is obtained by linear regressions from many different char types. Therefore, statistically the error with Eq. (12) could be smaller than that with experimental data just for one specific char type.

2.3. Heat transfer

For small char particles, which are mainly in pulverized coal boilers and partly in fluidized beds, it is reasonable that the temperature inside a particle is uniformly distributed. The heat released from the carbon combustion is balanced with the convection, radiation and heat absorbed by the char particle, or

$$\frac{mC_p^{(c)}}{4\pi r_s^2}\frac{\mathrm{d}T_\mathrm{p}}{\mathrm{d}t}+\varepsilon\sigma(T_\mathrm{p}^4-T_\mathrm{w}^4)+h(T_\mathrm{p}-T_\infty)=\frac{0.012Q}{4\pi r_s^2}H \tag{14}$$

The convection heat transfer coefficient, h, is calculated as

$$Nu=\frac{2hr_s}{\lambda_\mathrm{g}}=2 \tag{15}$$

2.4. Weight loss due to combustion

Let G be char consumption rate (kg m^{-2} s^{-1}), and

$$G=\frac{0.012Q}{4\pi r_s^2(1-\eta)} \tag{16}$$

The lifetime of the char particle is solved by

$$-\rho\frac{\mathrm{d}r_s}{\mathrm{d}t}=G \tag{17}$$

The detail of char particle combustion can be displayed by numerically solving Eqs. (4), (13), (14) and (17) simultaneously.

3. Results and discussions

In numerical simulations, a char particle is assumed to be injected into a bulk flow with high temperatures at the atmosphere pressure. The initial temperature of this single particle is 25 °C. The bulk flow temperature is simply assumed to be uniform. The numerical results are obtained at the bulk flow temperature 1273 and 1700 K respectively. Although the bulk flow temperature distributions employed are different from those in real boilers whose temperatures are not uniformly distributed, the results are still helpful in understanding single char particle combustion behavior. The mole concentration of oxygen at the bulk flow is 21%.

Several different types of char samples are used in the simulations. The numerical results for two typical char samples are shown in this paper. Other samples have the similar behaviors. The properties of these two char samples are listed in Tables 1 and 2.

3.1. Temperature profiles

Fig. 2 shows the temperature profiles of Yongcheng char for different initial particle diameters. It can be seen that small particles reach the environmental temperatures fast. However, after the environmental temperature is reached, the temperature profiles are quite different for various diameters. When the initial particle diameter is not larger than 175 μm, the particle temperatures are increased from the room temperature to a temperature that is higher than the environmental temperature a little bit. For the initial particle diameter larger than 180 μm, the particle temperature are increased from the room temperature to a temperature that is much higher than the environmental temperature, and be decreased to the environmental temperature later with the particle diameter becomes small due to

Table 1
Parent coal samples

Samples	Heating values (cal/g)	Proximate analysis (air dry basis)				Ultimate analysis (dry basis)			
		Inherent moisture (%)	Ash (%)	Volatile matter (%)	Fixed carbon (%)	C (%)	N (%)	O (%)	S (%)
Yongcheng (China)	6840	1.65	18.4	8.8	71.2	74.7	0.8	2.8	0.4
Luoyang (China)	6890	1.70	16.2	11.5	70.6	75.1	1.3	3.5	0.4

Table 2
Char parameters

Samples	S_I (m^2/g)	β	η (%)
Yongcheng	1.80	0.400	22
Luoyang	2.87	0.514	23

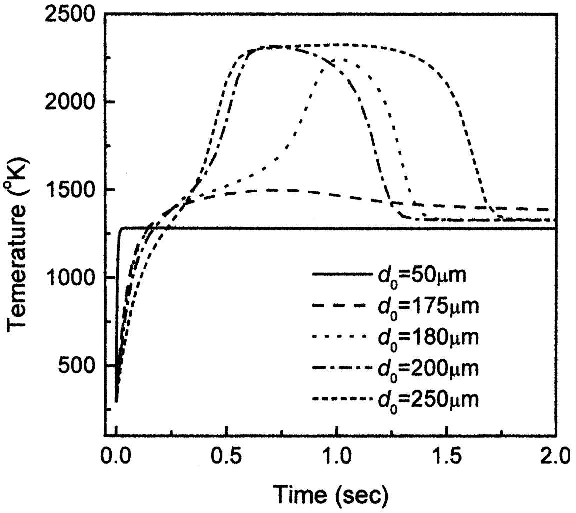

Fig. 2. Temperature profiles for different particle sizes (Yongcheng char; bulk flow temperature 1273 K).

combustion. The region of the initial diameter among 175–180 μm is a transition area.

Fig. 3 shows the oxygen concentrations at the particle surfaces for different initial diameters. The oxygen concentrations at the particle surfaces are not as the same as that in the bulk flow and are lower due to combustion. However, when the initial diameter is small, the oxygen concentration at the particle surface is quite close to the oxygen concentration at the bulk flow. Therefore, the char combustion is basically not affected by the oxygen diffusion from the bulk flow to the particle surface. The combustion is chemically controlled. When the initial size is large, there are deep "valleys" for oxygen concentration profiles. These deep valleys mean that the particles have large char burning rates. The combustion is a diffusion-controlled process, oxygen diffusing from the bulk flow to the particle surfaces. Comparing Fig. 2 with Fig. 3, there are strong coherence between the temperature "peak" shapes in Fig. 2 and the oxygen "valley" shapes in Fig. 3. Fig. 3 shows that combustion for a large particle has two periods: diffusion controlled combustion and chemically controlled combustion. When the particle is large, the combustion is controlled by diffusion. But, after a period of burning when the particle size becomes small, the combustion is chemically controlled.

The heat generating rates from char combustion for different initial particle diameters are shown in Fig. 4.

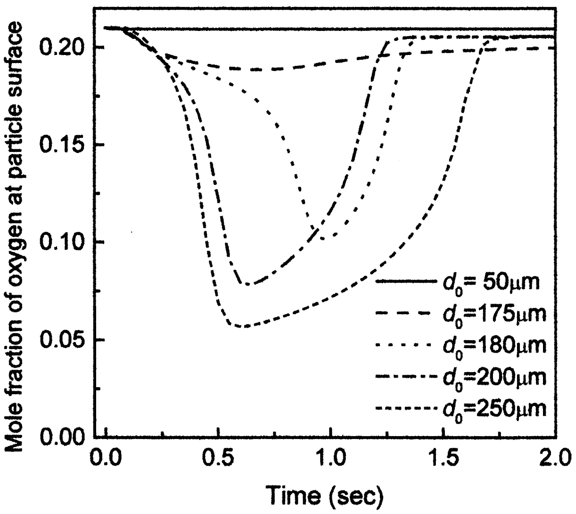

Fig. 3. The oxygen concentration at the particle surface (Yongcheng char; bulk flow temperature 1273 K).

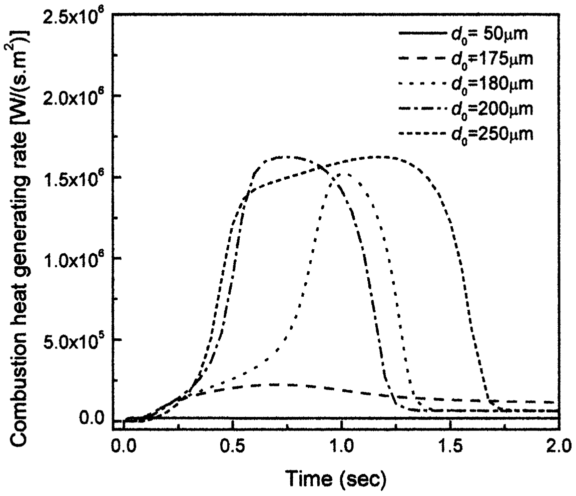

Fig. 4. Heat generating rates from char combustion (Yongcheng char; bulk flow temperature 1273 K).

From Fig. 4, the large particles either have high heat generating rates or hold long periods at high heat generating rates, which mean that the large particles either have high char combustion rates or hold long period at high char combustion rates. The similar observations for the convective heat transfer rates and radiative heat transfer rates can also be obtained. The higher convective heat transfer rates and radiative heat transfer rates for the larger particles are due to their higher temperatures at the large particle surfaces.

Fig. 5 shows the temperature profiles for Luoyang char. The diameter of the transition from diffusion

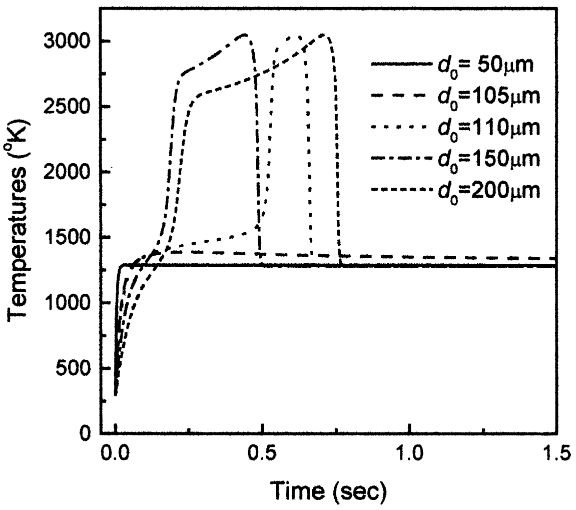

Fig. 5. Temperature profiles for different particle sizes (Luoyang char; bulk flow temperature 1273 K).

controlled combustion to chemically controlled combustion is different from that of Yongcheng char. In corresponding to the temperature profiles, other behaviors for Luoyang char combustion are similar to those in Yongcheng char combustion.

Fig. 6 shows the temperature profiles of Yongcheng char combustion with 1700 K bulk flow temperature. Comparing Fig. 2 with and Fig. 6, when the bulk flow temperature is increased, the initial particle size for combustion entering into diffusion controlled region becomes small.

From Eq. (4), the particle size affects the oxygen diffusion from the bulk flow to the particle surface. If the particle diameter is large, the oxygen diffusion rate from the bulk flow to the particle surface is large. Eq. (13) indicates that the particle size affects the particle reaction surface areas both in exterior and in interior. A large particle has large exterior surface area so that has large exterior chemical reaction surface area. Furthermore, the larger particle has bigger macro-pore surface areas in total, which are the main combustion surface areas. Therefore, the larger particle has bigger char combustion rate due to the larger combustion surface areas.

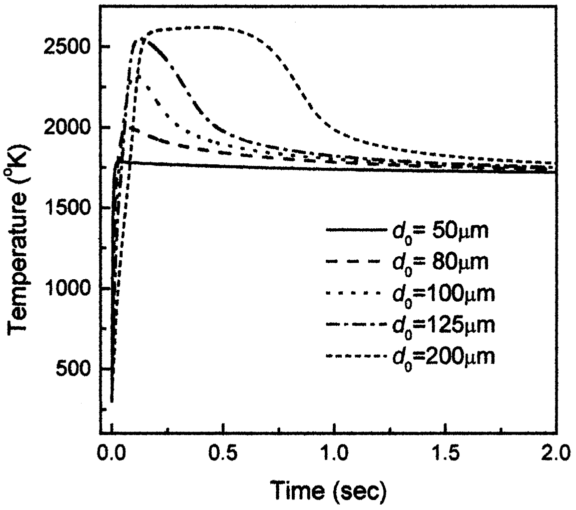

Fig. 6. Temperature profiles for Yongcheng char. The bulk flow temperature is 1700 K.

Eq. (15) shows that, compared with a small particle, the large particle has weak convective heat transfer coefficient. Hence, relatively the large particle has small convective heat transfer capability if the temperature difference is fixed. The larger particle also needs more heat to increase its internal energy.

Simply speaking, when the particle is large, the reaction surface areas (mainly porous surface areas) are large and the oxygen diffusion rate from the bulk flow to the particle surface is large. Then, more carbon is combusted and more reaction is generated. However, the convective heat transfer coefficient for large particle is small and the temperature is increased. On the other hand, the increased temperature further increases the combustion speed in turn. As a result, the particle temperature is risen to a high temperature, at which the quantity of transferred heat from the particle to the bulk flow is increased due to the increased temperature difference between the particle surface and the bulk flow.

For small particles, the transferred heat can be balanced to the generated heat from combustion at the low temperature difference. Therefore, Eq. (14) is satisfied at the low particle temperature that is close to the environmental temperature.

3.2. Carbon conversion profiles

Fig. 7 shows carbon conversions for Yongcheng char particles with different initial diameters. Apparently, there exists a critical value for the initial diameters between 175 and 180 μm. The temperature profiles in Fig. 2 also show the similar phenomena. When a char particle with a large initial diameter is burned and diminished into a small particle, the conversion rate is also changed. When the diameter is large, the conversion speed is fast. When the diameter is reduced below a certain value, the conversion speed is slow. This certain value is smaller than the critical value discussed at the last paragraph.

The combustion process can roughly be divided into two periods. When the particle is large, the combustion is under diffusion controlled combustion. When the particle is small, the combustion is under chemically controlled combustion.

Fig. 8 shows the time needed to 50% and 95% carbon conversion ratios for different initial diameters (Yong-

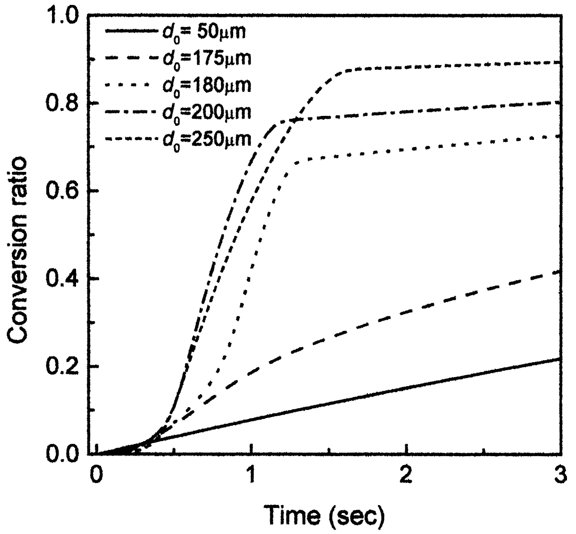

Fig. 7. Conversion profiles for different particle sizes (Yongcheng char; bulk flow temperature 1273 K).

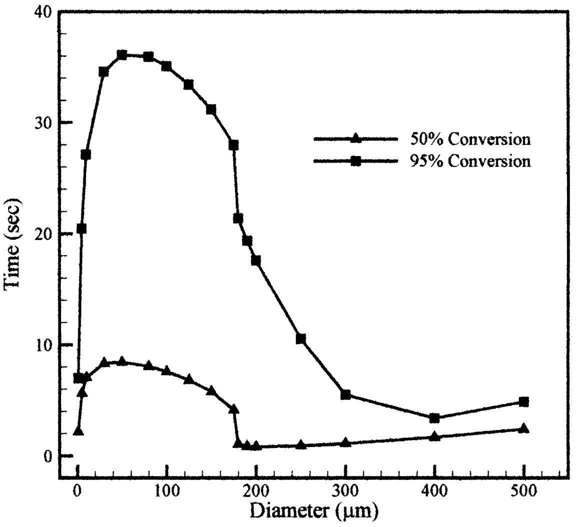

Fig. 8. The time needed to 50% and 95% conversion ratios for different initial diameters (Yongcheng char; bulk flow temperature 1273 K). Black points are calculated values.

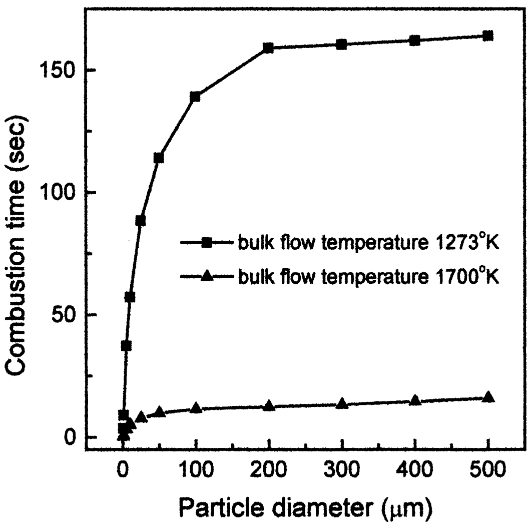

Fig. 9. Combustion time for different initial particle diameters when the char particle radiuses are diminished below 0.1 μm (Yongcheng char; bulk flow temperatures 1273 K and 1700 K). Black points are calculated values.

cheng char; 21% oxygen; bulk flow temperature 1273 K). It is widely accepted that small particles burn fast. However, Fig. 8 shows that, for single char particle combustion, there is optimized value for initial char particle diameters. Very small particles have relatively low conversion speeds.

In boiler designs, the combustion time is always an important issue. However, how to define the combustion time should be clarified. If the combustion time of a char particle is defined as the time needed when the radius of this particle is diminished to a fixed value, the following conclusion can be obtained: a smaller particle has less combustion time. Suppose the combustion time is defined as the time needed for the radiuses of the char particles being smaller than 0.1 μm in the combustion. Then, Fig. 9 shows very long combustion time for different initial particle diameters in Yongcheng char combustion for the bulk flow temperature of 1273 K. However, when the bulk flow temperature is increased to 1700 K, the combustion time will be reduced greatly, as Fig. 9 shows. This combustion time is still too long in practical applications. In boilers, the most widely used criterion in judging of combustion is the combustion efficiency. The carbon conversion ratio is more appropriate. Fig. 10 shows the combustion time for different initial diameters when the carbon conversion ratios are greater than 98% with the bulk flow temperature 1700 K. In this criterion, the combustion time is much smaller.

Consider a char particle with 80 μm diameter burning in 1600 °C (1873 K) bulk flow, which is close to the real situations in pulverized coal boilers. If the radius is diminished to 0.1 μm, the combustion time is 5.7 s. If the carbon conversion ratio is 98%, the combustion time is 1.86 s. In real pulverized coal boilers, the combustion time is about 2 s.

In coal combustion boilers the problem of unburned carbon in ash has been studied for a long time. The content of unburned carbon in ash for pulverized coal boilers is around 2%, unlike much high in fluidized beds. The above results have shown that this problem actually is an intrinsic property of char combustion. When char

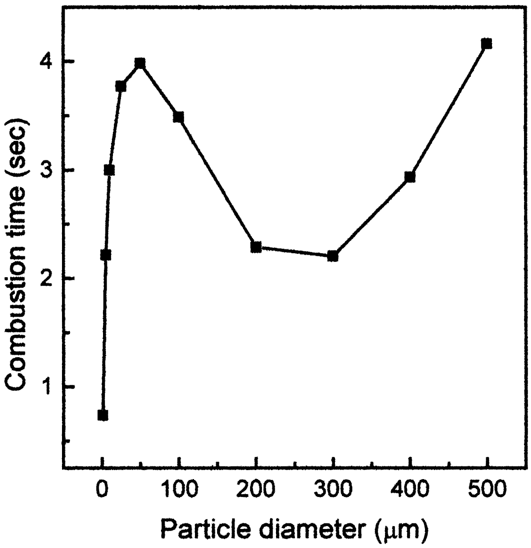

Fig. 10. Combustion time for different initial particle diameters when the carbon conversions are greater than 98% (Yongcheng char; bulk flow temperature 1700 K). Black points are calculated values.

particles become small in combustion, the carbon conversion speeds are low. No matter what kinds of measures are taken to enhance char combustion, it is impossible to completely burn out small char particles in power plant boilers in a limited period.

4. Conclusions

A one-dimensional char combustion model including pore structure effects is used to numerically investigate single char particle combustion. The numerical results for several different types of char samples show that the temperatures at the particle surface are quite different for various initial particle diameters due to the heat and mass transfer, together with combustion in pore surfaces. The larger particles in general have higher temperatures at the exterior surfaces. There are two ways to consider char combustion time. One is to consider the particle radius diminishing. Another is to consider the carbon conversion ratios. The later is more appropriate in practical applications. It is found that the size effects on char combustion are different for these two considerations. If just the particle radius is concerned, the small particles have less combustion time. But, if the carbon conversion ratio is concerned, there are optimal particle sizes in limited combustion time and smaller particles may have longer combustion time.

Besides in understanding of the heat transfer, mass transfer and reaction for single char particle combustion, the results presented in this paper have potential industrial applications. For power plants, coal particles are ground as small as possible. The idea is that small particles have better combustion efficiency in a limited burn period. On the other hand, the small particles need more grinding power and may defy high combustion efficiency economically. Usually, the particles are ground to about 80 μm diameter. This paper shows that, even if ignoring the grinding power, larger particles may have relative higher combustion efficiency. To each coal type, there exists a specific optimal particle diameter.

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