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Numerical investigation of different effects of carbon dioxide properties and carbon monoxide oxidation on char particle combustion in actual and fictitious O_2/CO_2 environments

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ABSTRACT

The overall and individual effects of carbon dioxide properties and carbon monoxide oxidation on char combustion were numerically simulated with a continuous-film model in different O_2/CO_2, O_2/N_2 and O_2/Ar environments, and different CO_2 physicochemical properties were artificially changed to distinguish the individual effect on char particle temperature and combustion rate. The results show that the char combustion rate in 21% O_2/79%CO_2 environment is slightly higher than that in air environment because of two opposite effects of higher char gasification reaction rate with high concentration CO_2 and lower char oxidation rate with O_2 resulting from lower particle temperature. At the same time, the CO flame front in 21%O_2/79%CO_2 environment is farther away from char particle surface than that in 21%O_2/79%N_2 environment because of lower diffusion coefficient of oxygen in CO_2 environment although the gas temperature is lower. Furthermore, the net effect of molar heat capacity of CO_2 on char combustion rate decreases and the net effect of char gasification reaction with CO_2 on char combustion rate distinctly increases with the increase of ambient gas temperature and O_2 mole concentration.

1. Introduction

The issue of carbon dioxide emission reduction during coal combustion process has become more and more important with the increasing global climate change, and oxy-fuel combustion is an economical option for carbon dioxide capture [1–3]. Oxy-coal combustion is greatly different from conventional pulverized coal combustion in air environment because of significant differences between CO_2 and N_2 properties [4,5]. The molar heat capacity of CO_2 is 1.7 times that of N_2 at the ambient gas temperature of 1400 K, and the diffusivity of O_2 in CO_2 environment is 0.8 times that in N_2 environment. In addition, high concentration CO_2 can participate in char combustion through char-CO_2 gasification reaction. Therefore, char particle combustion is one of the most important issues for oxy-coal combustion due to these different effects of carbon dioxide properties.

Different CO_2 effects on gas fuel combustion characteristics have been widely investigated with numerical simulation method. Guo et al. [6] adopted fictitious CO_2 method to numerically distinguish different effects of CO_2/N_2/Ar addition on liftoff of a laminar CH_4/air diffusion flame and demonstrated that the dilution effect on liftoff of flame is predominant followed by the thermal and chemical effects. Many investigators have paid more attention on the overall effect of CO_2 on char particle combustion rate because of the complex coal combustion process. However, the individual effects of CO_2 on char particle chemical reaction remain scarce because these effects are intimately coupled during coal char combustion process. Some researchers [7–9] demonstrated that the char particle temperatures were lower due to high molar heat capacity when N_2 was replaced by CO_2 at the same oxygen concentration. At the same time, the presence of CO_2 in O_2/CO_2 environment reduced the overall char particle reactivity because of high specific heat of CO_2 and slower oxygen diffusivity in O_2/CO_2 environment [10,11]. Thermal properties of CO_2 in O_2/CO_2 environment played an important role in the decrease of char combustion temperatures compared with O_2/N_2 environment [12], and char gasification reaction with CO_2 resulted in the effect of 25–33% on the char temperature decrease. Prationo et al. [13,14] modified the single-film model of coal combustion to investigate the effect of CO_2 and steam on coal ignition and char combustion rates, and illustrated that larger heat molar capacity of CO_2 than that of N_2 obviously delayed the coal ignition and the role of char gasification reaction was important for oxy-coal combustion. In order to quantitatively separate CO_2 effects on char combustion, Zhou et al. [15] proposed a numerical method to

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Nomenclature

C_P	specific heat (J/(kg·K))
D	diffusion coefficient (m^2/s)
Da	Damköhler number
E	activation energy (J/mol)
H	heat of reaction (J/kg)
k	reaction rate coefficient (m/s)
m	combustion rate (kg/s)
M	molecular weight (g/mol)
Q	stoichiometric carbon-to-CO reaction heat ratio
r	radial distance from carbon particle (m)
R_0	universal gas constant (J/(mol·K))
R	transient-to-initial radius ratio
t	time (s)
T	temperature (K)
w	reaction rate (kg/(m^2·s) or (kg/(m^3·s))
Y	mass fraction
ρ	density (kg/m^3)
υ	stoichiometric coefficient
ε	emissivity of particle surface
τ	non-dimensional time
θ	non-dimensional activation energy
σ	Stefan–Boltzmann constant (W/(m^2·K^4))
δ	product (CO_2)-to-carbon mass ratio
ξ	profile function

Subscripts

Ar	Ar
C	carbon
F	CO
g	gas
N	N_2
O	O_2
P	CO_2
S	particle surface
∞	ambience
0	initial state
1	reaction C + 1/2O_2 → CO
2	reaction C + CO_2 → 2CO

Superscript

~	dimensionless quantity

quantitatively separate different effects of CO_2 physiochemical properties by using Ar to replace an appropriate portion of CO_2 with a continuous-film model and indicated that the relative contributions of oxygen concentration, thermal, and chemical effects on the char combustion rate in O_2/CO_2 environment were 82.1%, 11.2%, and 6.7%, respectively. Zhang et al. [16] adopted the fictitious CO_2 properties to investigate the chemical and physical effects of CO_2 properties on coal ignition in O_2/CO_2 environment and demonstrated that the CO_2 chemical effect delayed coal ignition in O_2/CO_2 environment.

Moreover, carbon monoxide flame at the boundary layer of char particle has an important effect on char combustion because CO flame consumed a large amount of oxygen and prevented the oxygen diffusion towards char particle surface, which changed predominant surface reaction from char oxidation to char gasification [17]. Zhang and co-workers [18] established a moving flame front model to investigate the effect of carbon dioxide flame at the boundary layer on char combustion in O_2/N_2 environment, which was well verified by the continuous-film model. They demonstrated that CO flame front was formed at the particle surface under certain conditions. Gupta and co-workers [19,20] pointed out that char combustion regime was significantly affected due to the presence of CO flame at the boundary layer with a shrinking core model. Hecht et al. [21,22] analyzed the effect of char gasification reaction on coal combustion in O_2/CO_2 environment with SKIPPY model and concluded that char gasification reaction significantly reduced particle temperature, and CO flame was formed under higher oxygen concentration and char temperature. Yu et al. [23] pointed out that char burnout time was affected by the effect of CO oxidation under lower oxygen concentration and gas temperature. Gonzalo-Tirado et al. [24,25] adopted four different models to study the effect of CO flame at the boundary layer on char particle temperature and combustion rate and demonstrated that the single-film model is suited to the predictions in all cases and CO flame could promote the char combustion rate. The continuous-film model [26,27] simultaneously considers char oxidation and gasification and carbon monoxide oxidation reaction at the boundary layer to faithfully reflect char combustion process. Therefore, it can be regarded as an accurate benchmark to predict char combustion process in $O_2/CO_2/N_2$ environments [22–24,28].

Therefore, the objective of the present paper is to investigate the overall and individual effects of CO_2 properties and CO oxidation on char combustion in different O_2/CO_2, O_2/N_2 and O_2/Ar environments using the continuous-film model. The individual effects of CO_2 physiochemical properties on char combustion rates, including molar heat capacity of CO_2, oxygen diffusivity in CO_2 environment and char gasification reaction with CO_2, are numerically distinguished by using fictitious CO_2 method to elucidate different mechanisms of char combustion in O_2/CO_2 environment. In addition, the influencing factors on the location of CO flame front at the boundary layer of char particle are also analyzed to illustrate the effects of CO oxidation on char combustion in O_2/CO_2 environment.

2. Model

A spherical char particle burns in a quiescent environment at the ambient gas temperature of T_∞, and the main reactions in the continuous-film model include char surface oxidation with oxygen, char gasification reaction with carbon dioxide and gas-phase carbon monoxide oxidation reaction with oxygen. Carbon monoxide is regarded as the dominant product at the char surface due to higher particle temperature than 1100 K [27]. The detailed description of the continuous-film model can be found in references 15 and 27, and it is briefly introduced as following:

The char combustion rate $\widetilde{m} = m/(4\pi r_s \rho_\infty D_\infty)$ is defined as [27]

$$\widetilde{m} = \widetilde{m}_{C-O2} + \widetilde{m}_{C-CO2} = \left(Da_{S1}\frac{\widetilde{T}_\infty}{\widetilde{T}_S}\exp\left(-\frac{\theta_{S1}}{\widetilde{T}_S}\right)\widetilde{Y}_{O,S} + Da_{S2}\frac{\widetilde{T}_\infty}{\widetilde{T}_S}\exp\left(-\frac{\theta_{S2}}{\widetilde{T}_S}\right)\widetilde{Y}_{P,S}\right)/\delta \tag{1}$$

where $Da_s = k_s r_s/D_\infty$ is the surface Damköhler number, $\tilde{T} = \alpha_F c_P T/H_{CO}$, $\theta = \alpha_F c_P E/(R_0 H_{CO})$, $\tilde{Y}_O = \alpha_O Y_O$, $\tilde{Y}_P = Y_P$, $\delta = M_P/M_C$, $\alpha_F = \upsilon_P M_P/\upsilon_F M_F$, and $\alpha_O = \upsilon_P M_P/\upsilon_O M_O$.

The temporal variations of char particle temperatures and the radius are expressed by Eqs. (2) and (3) [15,27]

$$-\frac{\widetilde{c}_s}{3}R^2\frac{d\widetilde{T}}{d\tau} = -\left(\frac{d\widetilde{T}}{d\widetilde{r}}\right)_s + \widetilde{m}(1-\widetilde{c}_s)\widetilde{T}_S - QDa_{S1}\frac{\widetilde{T}_\infty}{\widetilde{T}_S}\exp\left(-\frac{\theta_{S1}}{\widetilde{T}_S}\right)\widetilde{Y}_{O,S} - QDa_{S2}\frac{\widetilde{T}_\infty}{\widetilde{T}_S}\exp\left(-\frac{\theta_{S2}}{\widetilde{T}_S}\right)\widetilde{Y}_{P,S} + \varepsilon R(\widetilde{T}_S^4 - \widetilde{T}_\infty^4)/B_O \tag{2}$$