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Mass transfer coefficients considering effects of steam in oxy-fuel combustion of coal char

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HIGHLIGHTS

- Modified mass transfer coefficients for gas reactants O_2, CO_2, and H_2O are derived.
- Great improvement is achieved by adding the correction factors into the model.
- Presence of steam has insignificant impacts on the mass transfer of O_2 and CO_2.
- Participation of O_2 and CO_2 reactions plays considerable role in H_2O mass transfer.
- More attention should be paid to the modification when O_2 oxidation is prevailing.

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ABSTRACT

Considering the effects of Stefan flow and steam in the oxy-fuel combustion of char, correction factors for the mass transfer coefficients of gas reactants, O_2, CO_2, and H_2O, are derived in the present work. By comparisons with the experimental data, the rigid continuous-film model, and the uncorrected single-film model, it is concluded that the corrections greatly improve the predictions of the particle temperature, combustion rates and burnout time. The correction factors are related to the gas components, reaction numbers and rate ratios. Generally, the increase of number and rate of surface reaction will result in the enhancement of Stefan flow and hence decrease the mass transfer coefficients. But discussion under the typical conditions of oxy-fuel combustion shows that different reaction has different impacts on the mass transfer of reactive gases. In the presence of steam, the correction for O_2 is nearly the same as cases neglecting the steam, owing to the low gasification rate of H_2O and the accelerative diffusion transfer of O_2 in H_2O and H_2. The correction for CO_2 increases slightly by about 3% because the gasification rate of H_2O is only a little higher than that of CO_2. On the contrary, the participation of O_2 and CO_2 reactions plays considerable role in the mass transfer coefficient of H_2O. Especially, the high rate reaction, like O_2 oxidation, has more remarkable effects on the mass transfer of gas reactants. Therefore, more attention should be paid to the modification of mass transfer coefficients when the O_2 oxidation reaction is prevailing in the char oxy-fuel combustion, for the transfer coefficients will be greatly changed.

1. Introduction

As one of the most attractive carbon capture technologies, oxy-fuel combustion for coal has won more and more attentions. Compared with the conventional coal combustion technology that uses air as oxidant, the feed gas in the oxy-fuel technology is the mixture of oxygen and recycled flue gas. Depending on the oxy-fuel combustion system applied (with either dry or wet re-circulated flue gas) [1,2], a high fraction of steam might be fed with the recycled flue gas. Besides, in the oxy-fuel combustion of lignite or biomass based fuels, water content within the flue gas is often quite high. For these cases, the char particles combust in a gas with higher contents of O_2, CO_2, and H_2O. The CO_2 and H_2O are not only the dilution agents of O_2, but also the reactants of carbon consumption, which is different from N_2 that is inert. A number of investigations have pointed out that the gasification effects of CO_2 and steam need to be considered for the oxy-fuel combustion [3–6].

The theory of gas–solid mass transfer has shown that strong Stefan flow can be formed at the solid surface due to the higher contents of reactive gas [7]. Only when the content of reactive gas is low enough, the calculation error for reaction rate can decrease to less than 10% [8]. Therefore, the Stefan flow is often neglected in the conventional pulverized coal combustion (O_2/N_2) due to lower contents of O_2, CO_2 and H_2O. But in oxy-fuel combustion where the reactive gases are enriched, the effects of Stefan

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Nomenclature

a	particle radius (m)
A	frequency factor (m/s or kg/(m^2 s Pa))
c	specific heat (J/(kg K))
C	correction factor (–)
D	diffusion coefficient (m^2/s)
Da	Damkohler number (–)
E	activation energy (J/mol)
g	molar flux per unit of area (mol/(m^2 s))
H	heat of reaction (J/kg)
k	reaction rate coefficient (m/s or kg/(m^2 s Pa))
k_D	mass transfer coefficient (kg/(m^2 s))
M	molecular weight (kg/mol)
p	pressure (Pa)
r	radial distance from carbon particle (m)
R	reaction rate per unit of surface area (kg/(m^2 s))
R_u	universal gas constant (J/(mol K))
S	external surface area (m^2)
t	time (s)
T	temperature (K)
w	dimensionless gas reaction rate (–)
W	mass of particle (kg)
y	molar fraction (–)
Y	mass fraction (–)
ε	emissivity of particle surface (–)
ϕ	dimensionless molar flux per unit of area (–)
φ	ratio of CO_2 diffusion to O_2 diffusion in a common environment (–)
λ	thermal conductivity (W/(mK))
ν	stoichiometric coefficient or reaction order (–)
ρ	density (kg/m^3)
σ	Stefan–Boltzmann constant (W/(m^2 K^4))
ξ	coordinate normalized by particle radius (–)

Subscripts

C	carbon
g	gas
p	constant pressure
s	surface
0	initial
∞	ambience

Superscript

0	surface
$\sim$	dimensionless quantity

flow on the mass transfer and reaction rate cannot be overlooked. Hayhurst [9] found that neglecting the Stefan flow can result in significant errors in some cases. For oxygen reacting with a carbon particle, he used a modified Sherwood number to account for the effects of Stefan flow. Essenhigh [10] also observed that neglect of the Stefan flow can bring 12% systematic error in mass transfer calculation for carbon–oxygen reaction. Förtsch [11] gave a correction factor to the baseline case of oxygen diffusing in a stagnant gas film with all binary diffusion coefficients being equal and neglecting Stefan flow. It is shown that the correction can be up to 17%, depending on the primary reaction product, reaction rate, and gas-phase composition. Authors [12] studied the effects of Stefan flow on the char combustion in O_2/CO_2 mixtures and found that the mass transfer coefficient of CO_2 gas is more sensitive to the influencing factors and the error will be 74% if Stefan flow is neglected. Besides the reaction products and ambience gas compositions, the mass transfer coefficients are also related to the reaction rate ratio of surface oxidation to the surface CO_2 gasification. Neglect of Stefan flow will inevitably bring great errors in predicting the consumption rate and the burnout time of char.

The studies above were carried out only for the mass transfer of O_2 or CO_2 and did not take the steam and its gasification reaction at the char surface into account. In the presence of steam, the effects of H_2O gasification on the mass transfer of O_2 or CO_2 are not clear. The mass transfer coefficients of O_2, CO_2, and H_2O considering the effects of Stefan flow also need to be provided to aid the understanding of char oxy-fuel combustion. Therefore, in the following sections, the modified mass transfer coefficients of gas reactants that consider the Stefan flow, are derived firstly and then verified by comparing the model predictions that use the modified mass transfer coefficients, with other combustion models and the experimental data. Finally, the effects of steam and surface reactions on the mass transfer coefficients are discussed under the typical conditions of oxy-fuel combustion.

2. Mass transfer coefficients

It is assumed that the char particle is a uniform sphere and is burned in a quiescent atmosphere. At temperatures higher than 1000 K, the dominant heterogeneous reactions at the particle's surface are as follows,

$$2C + O_2 \rightarrow 2CO \quad (R1)$$

$$C + CO_2 \rightarrow 2CO \quad (R2)$$

$$C + H_2O \rightarrow CO + H_2 \quad (R3)$$

If considering reactions R1, R2, and R3, and assuming that no homogeneous oxidation of CO and H_2 takes place around the char particle, the gas surrounding the particle is composed of O_2, CO_2, CO, H_2O, and H_2. Fig. 1 gives the schematic of char combustion and coordinate system.

The reaction rate of a certain reaction, $R_{s,C-i}$, can be defined as the rate of mass removal per unit of external surface area,

$$R_{s,C-i} = -\frac{1}{S}\frac{dW_{C-i}}{dt} = M_C g^0_{C,C-i}, \quad i = O_2, CO_2, H_2O \quad (1)$$

where M_C is the molecular weight of carbon and $g^0_{C,C-i}$ is the molar flux of carbon removed per unit of external surface area regarding this reaction.

The reaction rate is also related to the diffusion of reactive gas in the boundary layer that is proportional to the difference between the molar fractions of reactive gas in the main stream flow and at the particle's surface. So the reaction rate is also expressed as

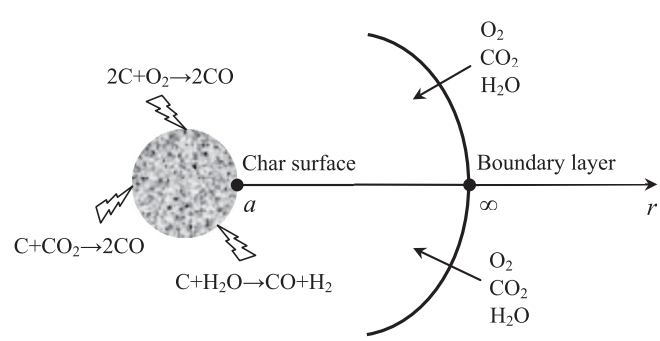

Fig. 1. Schematic of char combustion and coordinate system.