Combustion and Flame 161 (2014) 2177–2191

Contents lists available at ScienceDirect

Combustion and Flame

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

Analysis and modeling of char particle combustion with heat and multicomponent mass transfer

Hiroki Umetsu *, Hiroaki Watanabe, Shiro Kajitani, Satoshi Umemoto

Energy Engineering Research Laboratory, Central Research Institute of Electric Power Industry (CRIEPI), 2-6-1 Nagasaka, Yokosuka, Kanagawa 240-0196, Japan

ARTICLE INFO

Article history:
Received 25 October 2013
Received in revised form 15 January 2014
Accepted 28 January 2014
Available online 1 March 2014

Keywords:
Char
Combustion
Random pore model
Multicomponent
Dusty gas model

ABSTRACT

A char combustion model suitable for a large-scale boiler/gasifier simulation, which considers the variation of physical quantities in the radial direction of char particles, is developed and examined. The structural evolution within particles is formulated using the basic concept of the random pore model while simultaneously considering particle shrinkage. To reduce the computational cost, a new approximate analytical boundary condition is applied to the particle surface, which is approximately derived from the Stefan–Maxwell equations. The boundary condition showed reasonably good agreement with direct numerical integration with a fine grid resolution by the finite difference method under arbitrary conditions. The model was applied to combustion in a drop tube furnace and showed qualitatively good agreement with experiments, including for the burnout behavior in the late stages. It is revealed that the profiles of the oxygen mole fraction, conversion, and combustion rate have considerably different characteristics in small and large particles. This means that a model that considers one total conversion for each particle is insufficient to describe the state of particles. Since our char combustion model requires only one fitting parameter, which is determined from information on the internal geometry of char particles, it is useful for performing numerical simulations.

1. Introduction

Efficient coal combustion is strongly desired for the effective use of energy resources and the reduction of the cost of power generation. To meet these requirements, reducing the amount of unburnt carbon in fly ash is important because this enhances not only the combustion efficiency but also the value of the fly ash, which is obtained in large amounts as a by-product and has a high disposal cost. To reduce the amount of unburnt carbon, it is important to evaluate the temperature history of particles, their reaction rate, and other factors by numerical simulation, which is a useful tool for understanding phenomena that are difficult to measure in a full-scale boiler from the viewpoints of technical issues and cost. Many researchers are investigating the mathematical modeling on pulverized coal combustion and applying their models to the laboratory and practical-scale boilers (e.g. [1–9]). Kurose et al. [1,2] and Hashimoto et al. [3] applied RANS and LES based CFD to the bench-scale boilers and found that the unburnt carbon and NO emission could be qualitatively captured by their simple char combustion models with adjusting the kinetic parameters of heterogeneous reactions to the experimental data. Belosevic et al. [4] successfully applied RANS to the large-scale boiler to predict the temperature distribution and NO formation behavior. In these computations, the char combustion/gasification rate has a strong impact on state quantities and is one of the most important factors for obtaining an accurate prediction, since the char combustion/gasification is the rate-limiting reaction because heterogeneous reactions are typically much slower than homogeneous reactions in a boiler. However, simple char combustion models [10,11] are still used in the numerical analysis of large-scale boilers. The Field model [10] is the most successful model and is still the most frequently used for large-scale simulations [1–7]. Field considered the mass transfer resistance in a fluid film and expressed the transition from a controlled reaction to a diffusion-limited reaction by expressing the reciprocal of the apparent reaction rate as the sum of the reciprocals of the kinetic reaction and diffusion rates in his model. Smith [11] introduced the effectiveness factor, which accounts for the mass transfer resistance within a particle, in addition to the resistance in the fluid film in the Intrinsic model. Hurt et al. [12] reduced the likelihood of rapid burnout in the late stages of carbon conversion, which can be illustrated using the above two models, by introducing the ash film model, statistical kinetics, and thermal annealing in the CBK model. To take the effect of particle shrinkage into account, an empirical relation between diameter and density [12,13] (the burning mode, BM) is often used together

* Corresponding author. Fax: +81 46 856 3346.
E-mail address: umetsu@criepi.denken.or.jp (H. Umetsu).

http://dx.doi.org/10.1016/j.combustflame.2014.01.029
0010-2180/

Nomenclature

Roman symbols

a	pore radius (m)
a_r	mean pore radius (first moment of $f(a)$) (m)
$a_{r,0}$	initial mean pore radius (m)
A	pre-exponential factor (kg/m^3 Pa^n)
$\mathcal{B}$	coefficient matrix in terms of diffusion defined in Section 2.5 (m^2/s)
$\mathcal{B}^K$	coefficient matrix in terms of Knudsen diffusion defined in Section 2.5 (m^2/s)
$\mathcal{B}^M$	coefficient matrix in terms of molecular diffusion defined in Section 2.1 (m^2/s)
$\mathcal{B}^M_{ij,0}$	coefficient matrix in terms of molecular diffusion when $T = T_0$ and $x_i = x_{i,0}$ for all the species (m^2/s)
c	concentration (mol/m^3)
c_0	concentration when $T = T_0$ (mol/m^3)
c_p	specific heat per unit volume (J/m^3 K)
$c_{p,i}$	constant-pressure specific heat of species i (J/mol K)
$c_{p,i,0}$	constant-pressure specific heat of species i when $T = T_0$ (J/mol K)
c_s	concentration at surface of particle (mol/m^3)
$c_{v,\mathrm{Ash}}$	specific heat of ash per unit mass (J/kg K)
$c_{v,\mathrm{C}}$	specific heat of carbon per unit mass (J/kg K)
d_p	particle diameter (m)
D_{ij}	binary diffusion coefficient for species i through species j (m^2/s)
D^e_{ij}	effective binary diffusion coefficient for species i through species j (m^2/s)
$D_{i,\mathrm{Kn}}$	Knudsen diffusion coefficient of species i (m^2/s)
$D^e_{i,\mathrm{Kn}}$	effective Knudsen diffusion coefficient of species i (m^2/s)
e_r	energy flux (J/m^2 s)
E	activation energy (kJ/mol)
f	probability density function of pore axes
h	total enthalpy per mole (J/mol)
$\tilde{h}_i$	enthalpy of species i per mole (J/mol)
$\tilde{h}_{i,0}$	enthalpy of species i per mole when $T = T_0$ (J/mol)
h_V	total enthalpy per unit volume (J/m^3)
l	total length of pore axes per unit volume (m/m^3)
m	parameter of shrinkage
M_i	molecular weight of species i (kg/mol)
n	reaction order
N	flux including convection and diffusion (mol/m^2 s)
$\mathcal{N}$	number of shells
N_i	flux including convection and diffusion of species i (mol/m^2 s)
$N_{i,s}$	flux including convection and diffusion of species i at surface of particle (mol/m^2 s)
Nu	Nusselt number (–)
p	pressure (Pa)
Q_i	total flux of species i including convection and diffusion (mol/s)
Q_w	heat flux at wall (W/m^2)
r	radial position (m)
r_g	radial position at ambient side edge of fluid film (m)
r_s	radial position at surface of particle (m)
$r_{s,0}$	radial position at surface of particle at initial state (m)
R	gas constant (J/mol K)
R_i	reaction rate of species i per unit volume (mol/m^3 s)
s	surface area per unit volume (m^2/m^3)
s_0	surface area per unit volume at initial state (m^2/m^3)
s_c	surface area of carbon per unit volume (m^2/m^3)
$s_{c,0}$	surface area of carbon per unit volume at initial state (m^2/m^3)
t	time (s)
T	temperature (K)
T_0	mean temperature $(T_s + T_g)/2$ (K)
T_g	temperature at ambient side edge of fluid film (K)
T_s	temperature at surface of particle (K)
T_w	wall temperature (K)
v^*	mole-averaged velocity (m/s)
v^*_s	mole-averaged velocity at surface of particle (m/s)
x_i	mole fraction of species i (–)
$x_{i,0}$	mean mole fraction of species i $(x_s + x_g)/2$ (–)
$x_{i,g}$	mole fraction of species i at ambient side edge of fluid film (–)
$x_{i,s}$	mole fraction of species i at surface of particle (–)
X	total carbon conversion of char whose initial state was that after the pyrolysis experiment (kg/kg)
$\overline{X}$	$1 - X$
X_a	ash ratio in terms of volume (m^3/m^3)
$X_{a,0}$	initial ash ratio in terms of volume (m^3/m^3)
Y	number of gaseous species or species Y

Greek symbols

α_w	heat-transfer coefficient (W/m^2 K)
ϵ	emissivity (–)
λ	thermal conductivity (W/m K)
λ_0	thermal conductivity when $T = T_0$ and $x_i = x_{i,0}$ (W/m K)
λ_{Ash}	thermal conductivity of ash (W/m K)
λ_{C}	thermal conductivity of carbon (W/m K)
λ_i	thermal conductivity of species i (W/m K)
μ	viscosity (kg/m s)
Ψ	random pore model structural parameter
ρ_{Ash}	density of ash (kg/m^3)
ρ_{C}	density of carbon (kg/m^3)
σ_B	Stefan–Boltzmann constant (W/m^2 K^4)
τ	tortuosity (–)
θ	porosity (m^3/m^3)
θ_0	initial porosity (m^3/m^3)
$\bar{\theta}$	$1 - \theta$
θ_L	limit porosity (m^3/m^3)

with these models. These successful models define one carbon conversion for each particle. This means that the carbon conversion distribution in the radial direction is defined uniquely (uniform for the Field and Intrinsic models and in the form of a Heaviside step function for the CBK model), regardless of particle diameter. The reason for the selection of these models in previous studies is thought to mainly be for their usability and computational cost. However, the usability is achieved by making an adjustment of the model parameters to fit the conversions of simulation and experiment for each intended furnace, although the original model parameters which are determined by fundamental experiments (e.g., thermogravimetric analysis and drop tube furnace) should be used for any furnace. Very recently, Singer and Ghoniem have investigated char combustion [14,15] in detail by considering the pore distribution within a particle and its development for each pore size (adaptive random pore model). The model is fully predictive (without any fitting parameters) and gives accurate predictions. However, its computational cost and the many measurable/unmeasurable parameters make it difficult to apply the model to large-scale computations.