Analysis of pulverized coal flame stabilized in a 3D laminar counterflow

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ABSTRACT

In this paper, pulverized coal flames stabilized in a three-dimensional laminar counterflow configuration are simulated with detailed chemistry and the flame behaviors are analyzed in detail. Effects of radiation, coal particle mass flow rate and strain rate on the pulverized coal flame structure are investigated. The results show that the coal particles transported by the air stream tend to be ignited in a premixed combustion mode, which is followed by a non-premixed flame reaction zone, forming a typical double-flame type structure. The contribution of premixed combustion to the total heat release rate is sensitive to the studied operating conditions. Both volatile combustion and char off-gases combustion contribute to premixed combustion and their relative importance is influenced by the operating conditions. The pulverized coal combustion is significantly affected by radiative heat transfer. Without radiation, the reaction zone becomes thinner and the ignition is delayed. As the coal particle mass flow rate increases, the coal particles are ignited earlier and the combustion of char off-gases expands over a larger region. As the strain rate increases, both the premixed combustion share and the contribution of char off-gases combustion to the total heat release rate are decreased. For the extremely high strain rate case, the oxidizer can diffuse into the coal cloud from the oxidizer side to ignite the gas fuels at the fuel side (i.e. effect of oxidizer "leakage"). In order to properly consider the interphase heat transfers in gaseous flamelet models, a new tabulation method (compared to the conventional ones, e.g., Wen et al., (2017)) is proposed. The *a priori* analysis of the new tabulation method on different configurations shows that, compared to the conventional tabulation method, it better accounts for the heat transfers between the coal particle phase and gas phase, and can be applied to combustion systems with different oxidizer streams without introducing additional manifolds.

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1. Introduction

Coal has been and will continue to be one of the major energy resources in the near future in some countries (e.g. China, Germany and Russia) because of its abundant reserves and competitively low prices [1]. However, pulverized coal-fired power plants represent significant sources of pollutants, including NO_x, SO_x, CO_2, etc. Efforts are therefore required to make the use of coal more efficient and environmentally acceptable, motivating the coal combustion research. Since the maximum temperature of pulverized coal flame exceeds 1800 K, some substances (e.g. radical species) are hardly measured [2]. Computational fluid dynamics (CFD) has become an important tool to describe the pulverized coal combustion behaviors [3–7]. However, since pulverized coal combustion is an extremely complex phenomenon, in which the dispersion of highly reactive solid particles, evaporation, devolatilization, char surface reactions, and volatile and char off-gases combustion take place interactively and strongly interact with turbulence and radiation, the underlying physics governing the process of pulverized coal combustion have not been well understood. Simple models with strong assumptions, e.g., single-step chemical reaction mechanism, infinitely fast chemistry, over-simplified volatile matter composition, etc, were often used in previous works [3–7]. In these studies, the thermo-chemical quantities were not well predicted as expected.

Despite of the above-mentioned complexities, some progresses have been made for modelling pulverized coal combustion with more advanced models [8–21], among which the flamelet models [22] were extensively studied over the past three years [8–15] since they can take detailed chemistry mechanism into account without a high computational cost. Although the predicted

Nomenclature

Variables

A_1	Pre-exponential factor in the devolatilization model, 1/s
A_s	Particle surface area, m^2
$A_{p,i}$	Volumetric particle projected area, m^2
C_1	Mass diffusion limited rate constant, s/K$^{0.75}$
C_2	Kinetics limited rate pre-exponential constant, 1/s
C_D	Drag coefficient
$C_{p,ash}$	Specific heat capacity of ash, J/(kg K)
$C_{p,char}$	Specific heat capacity of char, J/(kg K)
$C_{p,g}$	Specific heat capacity of gases, J/(kg K)
$C_{p,p}$	Coal particle specific heat capacity, J/(kg K)
$C_{p,p}^0$	Initial coal particle specific heat capacity, J/(kg K)
$C_{p,vol}$	Specific heat capacity of volatile matter, J/(kg K)
D_k	Mass diffusivity of the species k, m^2/s
d_p	Particle diameter, m
E	Activation energy in the devolatilization model, J/mol
E_k	Kinetics limited rate activation energy, J/mol
E_p	Emission contribution of the coal particles, W/m^3
FI	Flame index
g_i	Gravity acceleration in the ith direction, m/s^2
H_e	Specific total enthalpy, J/kg
$L_{vol,k}$	Latent heat of species k, J/kg
LHV_k	Lower heating value of species k, MJ/kg
m_p	Mass of a single coal particle, kg
m_p^0	Initial mass of coal particle, kg
$m_{char,k}$	Mass of species k in the char surface reactions, kg
m_{char}	Mass of char, kg
$m_{vol,k}$	Mass of species k in the volatile matter, kg
m_{vol}	Mass of volatile matter, kg
N	Number of coal particles per second
Nu	Nusselt number
p	Static pressure, Pa
P_{cg}	Parameter P_{cg}
Pr	Prandtl number
Q	Q-factor in the devolatilization model
q_m	Coal particle mass flow rate, kg/s
Q_{char}	Heat source due to char-oxidation, J/kg
R	Universal gas constant, J/(mol K)
Re_p	Particle's slip Reynolds number
$\dot{S}_r$	Temperature source term due to devolatilization and char-oxidation, W
$\dot{S}_{C,He}$	Source term in total enthalpy conservation equation, J/(m^3 s)
$\dot{S}_{C,m,k}$	Source term in mass fraction conservation equation, kg/(m^3 s)
$\dot{S}_{C,m}$	Source term in mass conservation equation, kg/(m^3 s)
$\dot{S}_{C,u_i}$	Source term in momentum conservation equation, kg/(m^2 s^2)
$\dot{S}_{rad,g}$	Radiative heat exchange between coal particle and gas phase, W
$\dot{S}_{rad,p}$	Particle radiation source term, W
s_p	Equivalent particle scattering coefficient, 1/m
SR	Strain rate, 1/s
T	Gas temperature, K
T_p	Particle temperature, K
T_{dev}	Devolatilization temperature, K
u_i	Gaseous phase velocity in the ith direction, m/s
$u_{p,i}$	Particle velocity in the ith direction, m/s

u_{rel}	Relative velocity between gas and particle, m/s
W_β	Molar weight of the volatiles ($\beta = vol$) or char ($\beta = char$), kg/mol
W_{O_2}	Molecular weight of O$_2$, kg/mol
Y_k	Mass fraction of species k
Y_{ash}	Fraction of ash in the coal particle
Y_{ash}^*	Fraction of ash initially present in the particle
Y_{char}	Fraction of char in the coal particle
Y_{char}^*	Fraction of char initially present in the particle
$Y_{vol,k}$	Fraction of species k in the volatile matter
Y_{vol}	Fraction of volatile matter in the coal particle
Y_{vol}^0	Fraction of volatile matter obtained by proximate analysis
Y_{vol}^*	Fraction of volatile matter initially present in the particle

Greek symbols

α	Thermal diffusivity, m^2/s
α_g	Absorption coefficient of the gray gas, 1/m
α_p	Equivalent coal particle absorption coefficient, 1/m
$\Delta\xi_{pro}$	Mass consumption of char off-gases in the local cell between discrete time steps, kg
$\Delta\xi_{vol}$	Mass consumption of volatile matter in the local cell between discrete time steps, kg
δ_{ij}	Kronecker delta function
$\dot{\omega}_k$	Reaction rate of the species k, kg/(m^3 s)
$\dot{\omega}_T$	Heat release rate, J/(m^3 s)
$\dot{\omega}_{PV}$	Production rate of progress variable, kg/(m^3 s)
ϵ	Vanishingly small positive number
$\eta_{FI,\beta}$	Contribution of volatile/char combustion to premixed/non-premixed combustion
Γ	Exchange coefficient, m
γ	Particle volume fraction
λ	Thermal conductivity, W/(m K)
μ	Dynamic viscosity, kg/(m s)
ρ	Gaseous phase density, kg/m^3
ρ_p	Particle density, kg/m^3
ρ_p^0	Initial particle density, kg/m^3
σ	Stefan-Boltzmann constant, W/(m^2 K^4)
$\sigma_{p,i}$	Particle scattering factor
τ_d	Particle relaxation time, s
$\varepsilon_{p,i}$	Emissivity of the ith particle
ϑ_{st}	Stoichiometric oxygen mass fraction required for char-oxidation
ξ_{pro}	Mass of gas originating from the char off-gases, kg
ξ_{vol}	Mass of gas originating from the volatile matter, kg
ζ	Fraction of heat retained by particle due to char-oxidation

Abbreviations

CFD	Computational fluid dynamics
FVM	Finite volume method
HRR	Heat release rate

results have been improved, there still exist discrepancies between the model predictions and the experimental measurements in these studies. This can be attributed to the fact that the complicated operating conditions such as radiative heat transfer, coal particle mass flow rate, strain rate, etc, were neglected or determined empirically in these extended flamelet models. For example, the radiative heat transfer between the coal particle phase and gas phase was generally approximated by lowering the temperature on the fuel side of the flamelet equations while keeping the temperature on the oxidizer side constant [8–11]. However, this may not be true since, on the one hand, the cold coal particles (i.e. fuel side)