International Journal of Multiphase Flow 000 (2018) 1–15

Contents lists available at ScienceDirect

International Journal of Multiphase Flow

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

Large-eddy simulation of multiphase combustion jet in cross-flow using flamelet model

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ARTICLE INFO

Article history:
Received 11 February 2018
Revised 26 May 2018
Accepted 19 June 2018
Available online xxx

Keywords:
Pulverized coal combustion
Flamelet model
Flame-flame interactions
Wall heat losses
Jet in cross-flow

ABSTRACT

In this work, large-eddy simulations of pulverized coal combustion are conducted using the flamelet model, in which the devolatilization, char surface reactions, radiation and flame-wall interactions (FWI) are all considered. The mixings between the oxidizer and the volatiles/char off-gases are described with two mixture fractions Z_{vol} and Z_{char}, while the interphase heat transfer and progress of reactions are described with the manifolds of total enthalpy H_e and reaction progress variable Y_{PV}, respectively. The turbulence-chemistry interactions are considered with the presumed probability density functions. Standard pulverized coal combustion submodels are used to characterize the coal combustion sub-processes of devolatilization, char surface reactions, radiation, etc. Characteristics of pulverized coal combustion jet in cross-flow (JICF) are analyzed in detail. Particularly, the effects of the flame-flame interactions (FFI) and the wall heat losses (WHL) on the pulverized coal flame structure and thermo-chemical quantities distributions are studied through both qualitative and quantitative analyses. The results show that the overall flame temperature with twin jets in cross-flow (TJICF) is higher than that with single jet in cross-flow (SJICF) due to the FFI. The gas velocities in different directions have different sensitivities to the FFI, and the particle residence time/trajectory is influenced by the FFI. Three stages of FFI are identified, i.e., separated flames, merging flames and a merged flame. When the effects of WHL are neglected, the flame front becomes more wrinkling, the flame base moves towards the injectors, and the coal particles are ignited earlier. The pulverized coal flame structure at the lee-side of the flame front is more complicated than that at the leading-edge due to the different flow dynamics, and many burning pockets can be observed at the lee-side.

1. Introduction

Pulverized coal combustion is expected to remain a major source of electricity generation in many countries as coal reserves are much more abundant than those of other fossil fuels (Shaddix, 2012). In most pulverized coal-fired power plants, a tangential firing method is adopted due to its advantages of combustion stability, wide coal adaptability, and high combustion efficiency. However, the underlying physics governing the pulverized coal combustion processes in such systems are still not well understood. Since the temperature in the furnace is extremely high, experiments are difficult to conduct to provide reliable information (Kurose et al., 2009). Computational fluid dynamics (CFD) has become a powerful tool to describe pulverized coal combustion because it can provide detailed information of the distributions of temperature, species concentrations, etc. over the entire computational field (Wen et al., 2018, 2017a, 2017b, 2017c; Rieth et al., 2017; Messig et al., 2017; Watanabe et al., 2017; Stein et al., 2013; Stöllinger et al., 2013).

To date, simulations performed in the industrial furnace mainly employed the RANS (Reynolds-averaged Navier Stokes) approach due to its affordable computational cost. However, it is well-known that the unsteady motions which are important to flame dynamics cannot be predicted by RANS simulations. Large-eddy simulation (LES), on the other hand, offers many advantages when compared to the RANS technique in which large-scale flow structures are resolved and the unsteady flame behaviours are captured. Since the pioneering work conducted by Kurose and Makino (2003), significant progresses on LES of jet pulverized coal combustion have been made in recent years (Wen et al., 2017a; Rieth et al., 2017; Watanabe et al., 2017; Stein et al., 2013).

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https://doi.org/10.1016/j.ijmultiphaseflow.2018.06.017
0301-9322/

Nomenclature

Variables

A_c	Pre-exponential factor in char-oxidation model
A_s	Particle surface area
A_v	Pre-exponential factor in devolatilization model
C_D	Drag coefficient
$C_{p,\,g}$	Specific heat of gas phase
$C_{p,\,p}$	Specific heat of coal particle
D	Scalar molecular diffusivity
d_p	Particle diameter
D_T	Subgrid eddy diffusivity
E_c	Activation energy in char-oxidation model
E_v	Activation energy in devolatilization model
G	Incident radiation
g_i	Gravity acceleration
H_e	Total enthalpy
$H_{e,\,norm}$	Normalized total enthalpy
L_{vol}	Latent heat of volatile matter
m_p	Mass of a single coal particle
m_p^0	Initial mass of a single coal particle
M_X	Molecular weight of species X
m_{char}	Mass of char off-gases
m_{vol}	Mass of volatile matter
n	Number of particle in the local cell
Nu	Nusselt number
p	Static pressure
Pr	Prandtl number
Q	Factor used to consider the higher heating rate
Q_{char}	Heat source due to char-oxidation
Re_p	Particle's slip Reynolds number
$\dot{S}_r$	Temperature source term due to devolatilization and char-oxidation
$\dot{S}_{C,X}$	Two-way coupling term
S_{ij}	Strain rate
Sc_T	Subgrid Schmidt number
Sd	Separation distance between burners
T	Gas temperature
T_f	Temperature on the fuel side of flamelet
T_p	Particle temperature
T_{ox}	Temperature on the oxidizer side of flamelet
u	Gas phase velocity
u_p	Particle velocity
V	Grid cell volume
X	Mixing parameter
$Y_{pro,\,k}$	Fraction of species k in char off-gases
Y_{PV}	Reaction progress variable
$Y_{vol,\,k}$	Fraction of species k in volatile matter
Y_{vol}^*	Fraction of volatile matter initially in the coal particle
Z	Coal particle mixture fraction
Z''^2	Mixture fraction variance
Z_{char}	Char off-gases mixture fraction
Z_{vol}	Volatile matter mixture fraction

Greek symbols

α_g	Absorption coefficient of the gray gas
χ	Scalar dissipation rate
δ_{ij}	Kronecker delta function
ϵ	A small positive number (10^{-6})
μ	Dynamic viscosity
μ_T	Subgrid eddy viscosity
ρ	Gas phase density
ρ_p	Particle density
σ	Stefan–Boltzmann constant
τ_d	Particle relaxation time
ε_p	Particle's emissivity
ς	A model constant
ξ_{ox}	Mass of gas originating from the oxidizer stream
ξ_{pro}	Mass of gas originating from the char off-gases
ξ_{vol}	Mass of gas originating from the volatile matter
ζ	Fraction of heat retained by particle due to char-oxidation

Abbreviations

CFD	Computational fluid dynamics
CVP	Counter-rotating vortex pair
DNS	Direct numerical simulation
FFI	Flame-flame interactions
FGM	Flamelet-generated manifold
FPV	Flamelet/progress variable
FVM	Finite volume method
FWI	Flame-wall interactions
ILDM	Intrinsic low dimensional manifold
JICF	Jet in cross-flow
JPDF	Joint probability density function
LES	Large-eddy simulation
LES	Large-eddy simulation
LIF	Laser-induced fluorescence
PPDF	Presumed probability density function
RANS	Reynolds-averaged Navier Stokes
SGS	Subgrid-scale
SJICF	Single jet in cross-flow
TCI	Turbulence-chemistry interactions
TJICF	Twin jets in cross-flow
WHL	Wall heat losses

To predict the pollutants with slow chemistry time-scales such as NO_x, SO_x, etc, detailed chemical reaction mechanisms with finite rate chemistry are required, which may involve large numbers of species and reactions. Solving problems with such complex chemical reaction schemes in turbulent combustion is challenging for the following reasons (Poinsot and Veynante, 2005): (i) the transport coefficients and chemical reaction rates are complex functions of species mass fractions and temperature, which introduces uncertainties in their evaluations; (ii) the governing equation for each species should be solved, which results in high computational cost. Various approaches have been proposed to reduce chemical schemes, such as intrinsic low dimensional manifold (ILDM) method (Maas and Pope, 1992), flamelet tabulation method (Peters, 1984; Pierce and Moin, 2004; Van Oijen et al., 2001), etc. These reduction methods are promising since they take detailed chemical reaction mechanism into account with a reasonable computational cost. Various flamelet models have been developed to simulate gaseous (Pierce and Moin, 2004) and multiphase combustion (Ruggirello et al., 2012; Pandal et al., 2018; Wen et al., 2018, 2017a, 2017c; Rieth et al., 2017; Messig et al., 2017; Watanabe et al., 2017). Particularly, the flamelet tabulation models for pulverized coal combustion have been commonly used in recent years (Wen et al., 2018, 2017a, 2017c; Rieth et al., 2017; Messig et al., 2017; Watanabe et al., 2017). The flamelet concept for coal combustion was first used to predict single coal particle ignition by Vascellari et al. (2013). Similar work was conducted by Knappstein et al. (2016) using a so-called flamelet-generated manifold (FGM) model (Van Oijen et al., 2001). Watanabe and Yamamoto (2015) for the first time coupled the flamelet approach with a coal combustion model in the context of direct numerical simulation (DNS), in which both the devolatilization and char surface reaction processes were considered. Recently, they extended

Please cite this article as: X. Wen et al., Large-eddy simulation of multiphase combustion jet in cross-flow using flamelet model, International Journal of Multiphase Flow (2018), https://doi.org/10.1016/j.ijmultiphaseflow.2018.06.017