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Short communication

A DNS study on effect of coal particle swelling due to devolatilization on pulverized coal jet flame



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1. Introduction

Recently, a number of large-eddy simulations (LES) (e.g., [1-7]) and direct numerical simulations (DNS) (e.g., [8]) have been applied to pulverized-coal combustion fields, and the combustion mechanism and modelling have been discussed. However, in most of these previous studies, the effects from the changes in coalparticle diameter due to swelling and shrinkage during devolatilization and char combustion (e.g., [9-11]) on combustion characteristics have been neglected because of the lack of a specific model. The purpose of this study is, therefore, to investigate the effects of particle swelling and shrinkage during devolatilization and char combustion on the flame characteristics by performing DNS of a lab-scale turbulent pulverized-coal straight-jet flame [12]. A model for this purpose is proposed based on previous papers [9,10].

2. Numerical simulation

The governing equations for the gas phase are the conservation equations of mass, momentum, energy, mass of each chemical species *k*, and the equation of state for the ideal gas:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = S_{\rho},\tag{1}$$

ABSTRACT

The effects of particle swelling and shrinkage during devolatilization and char combustion on the flame characteristics are investigated by performing DNS of a lab-scale turbulent pulverized-coal straight-jet flame. The obtained characteristics are compared with those in the previous DNS (Hara et al., 2015), in which particle swelling and shrinkage are not taken into account. The results show that the changes in coal-particle diameter because of swelling and shrinkage during devolatilization and char combustion do not affect significantly the gas temperature distribution of the turbulent pulverized-coal straight-jet flame, although it explicitly affects the coal-particle diameter distribution in the flame.

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$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \boldsymbol{u}) = -\nabla P + \nabla \cdot \boldsymbol{\sigma} + S_{\rho \boldsymbol{u}},\tag{2}$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \boldsymbol{u}) = \nabla \cdot (\rho D_h \nabla h) + q_{\text{rad}} + S_{\rho h}, \tag{3}$$

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho Y_k \boldsymbol{u}) = \nabla \cdot (\rho D_k \nabla Y_k) + S_{\text{comb},k} + S_{\rho Y_k}, \tag{4}$$

$$P = \rho RT. \tag{5}$$

Here, ρ is the density, **u** the gas velocity, *P* the pressure, **o** the viscous stress tensor, h the specific enthalpy, D_h the diffusion coefficient of enthalpy $(=\lambda/\rho C_n)$, Y_k and D_k the mass fraction and the diffusion coefficient for chemical species k, R the gas constant, and T the gas temperature. In this study, D_k is given under the unity Lewis number assumption as $D_k = D_h$. Also, q_{rad} is the source term for radiation heat transfer and is calculated by the discrete ordinate method (DOM)/S4 [13] with a coefficient of absorption obtained by the weighted sum of gray gases (WSGG) [14], and $S_{\text{comb},k}$ is the source term for the combustion reaction of chemical species k. $S_{\rho}, S_{\rho u}, S_{\rho h}$ and $S_{\rho Y_{k}}$ are the source terms describing the phase coupling between the gas and dispersed-coal phases calculated using a particle-source-in-cell (PSI-Cell) model [15]. The pulverized-coal particles are tracked in the Lagrangian manner using the equation of motion for dispersed particles. The reaction models for coal combustion that we adopted can be found in Hara et al. [8] For the initial coal-particle diameter distribution, a Rosin-Rammler distribution with a number-averaged diameter of 25 µm and a mass-averaged diameter of 33 µm was chosen. The coal particle swells in the devolatilization dominant region and thereafter it begins to shrink because of the char combustion. Fig. 1 shows the



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Fig. 1. (a) Probability density function (PDF) of initial coal particle diameter, D_{p0} , and (b) variations of particle diameter, D_p/D_{p0} , against carbon conversion, *CV*, for Newlands coal at P = 0.1 MPa [9,10].



Fig. 2. Comparisons of (a) instantaneous distributions of particle position and diameter together with gas temperature, *T*, on central section, and (b) probability density function (PDF) of D_p at four streamwise locations (x = 30, 60, 90, 120 mm and r = 2 mm), between non-varying D_p and varying D_p cases.

probability density function (PDF) of initial coal particle diameter, D_{p0} , and variations of particle diameter, D_p/D_{p0} , against carbon conversion, *CV*, for Newlands coal at P = 0.1 MPa [9,10]. Based on Fig. 1 (b), an approximate expression of D_p/D_{p0} can be proposed as a function of *CV* by

$$D_{p}/D_{p0} = \begin{cases} 1+4.252CV-38.29CV^{2}+216.4CV^{3} \\ -586.2CV^{4}+593.0CV^{5} \\ -19.24-217.9CV-934.7CV^{2}+2090CV^{3} \\ -2576CV^{4}+1661CV^{5}-438.4CV^{6} \\ \end{cases} (CV \ge 0.35).$$
(6)

$$CV = 1 - \frac{X_c}{X_{c0}},\tag{7}$$

where X_c is the mass fraction of carbon content in each particle and X_{c0} is the initial mass fraction of carbon content in each particle.

The computational domain and other inlet boundary conditions for the turbulent pulverized-coal straight-jet flame are the same as given in Hara et al. [8]. The DNS was performed using a thermal flow analysis code: an in-house code referred as FK^3 [8,16,17]. The CPU time is about 0.37 million hours for each case on SGI:ICE X (1024 cores) at the Central Research Institute of Electric Power Industry.

3. Results and discussion

Fig. 2 shows the comparisons of instantaneous distributions of particle position and diameter together with gas temperature, *T*, on the central section, and PDF of D_p at four streamwise locations (x = 30, 60, 90, 120 mm and r = 2 mm), between non-varying D_p and varying D_p cases. Hereafter, we refer to the simulations without and with considering swelling and shrinkage effects on D_p as the non-varying D_p case and the varying D_p case, respectively.

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