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Numerical simulation of ignition in pulverized coal combustion with detailed chemical reaction mechanism

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ABSTRACT

A two-dimensional direct numerical simulation with a detailed chemical reaction mechanism that considers 158 species and 1804 reactions is applied to pulverized coal combustion occurring in a mixing layer and the ignition phenomena is investigated in detail. The pulverized coal particles which are initially heated up to 2000 K are distributed in a fully developed mixing layer. The distributions of temperature and various chemical species concentrations in terms of the mixture fraction are analyzed during ignition. The results show that the ignition occurs in the rich mixture fraction condition ($\xi \sim 0.2$), as the gas temperature is also high in this condition because of the high initial temperature set for the central coal particles. However, once ignition occurs, the combustion reaction dramatically takes place in the condition indicating $\xi = 0.03–0.06$, which is a slightly lean value compared with the stoichiometric value and shows the shortest ignition delay time in the calculation for autoignition of homogeneous mixtures of volatile matter and air (zero-dimensional calculation). In addition, in the combustion reaction zone, high OH radical mass fraction is observed around the conditions of stoichiometric mixture fraction, whereas high CH radical mass fraction is observed in the rich mixture fraction conditions.

1. Introduction

Coal is internationally the primary energy source because of its low procurement costs attributed to the large amount of recoverable reserves, widespread reserves, and stable supply. However, because coal-fired power generation produces large amounts of pollutants, such as SO_x (sulfur oxide) and NO_x (nitrogen oxide), it is important to improve the efficiency and to reduce the burden on the environment if we wish to continue using coal as a major source of energy in the future. The combustion process that occurs within the pulverized coal boiler is extremely complex as it involves several elementary processes such as the dispersion of particles in the flow field, heat transfer between the particles and the air surrounding them, release of flammable gases (volatile matter) from the particles, solid-state reactions, and gas-phase reactions, all of which are greatly affected by turbulence. Because of this complexity, employing numerical simulations is very helpful in designing and developing furnaces efficiently to obtain details that cannot be obtained from experiments (e.g., flow, temperature and concentration fields, and the behavior of the pulverized coal particles).

Recent computational fluid dynamics methods such as Reynolds-averaged Navier-Stokes (RANS) simulation (e.g., [1]), large-eddy simulation (LES, e.g., [1–10]) and direct numerical simulation (DNS, e.g., [11,12]) for the carrier gas have been applied to coal combustion and have revealed certain advantages of LES and DNS over RANS simulation in predicting local distributions of chemical species concentrations and gas temperature. In particular, to investigate ignition phenomena in gas and spray flames, DNS using the detailed chemical reaction mechanism is essential, and has been performed by many researchers (e.g., [13,14] for the gas flames and [15,16] for the spray flames). Although there are a few recent studies on the ignition phenomena in pulverized coal flame, they employ reduced chemical mechanisms (e.g., [17] for two-dimensional and [18–21] for three-dimensional).

The purpose of this study is, therefore, to obtain physical insight into the chemical reaction in an ignition of mono-dispersed pulverized coal particle-laden flow using two-dimensional numerical simulation with detailed chemical reaction mechanism. It should be noted that we refer the present two-dimensional numerical simulation, in which only the carrier gas is solved without any turbulence model, as two-dimensional DNS in the following.

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2. Numerical methods

The numerical methods for the present two-dimensional DNS are basically the same as those in Hara et al. [11] and Muto et al. [12] except for the reaction model of volatile matter and air mixture. The governing equations for the two-dimensional DNS of the gas phase are the conservation equations of mass, momentum, energy, mass fraction of each chemical species, and the equation of state for the ideal gas. On the other hand, the equations for the dispersed phase (coal particles) are the equations of each coal particle's position, x_p, velocity, u_p, temperature, T_p, and mass, m_p, as

$$\frac{d\boldsymbol{x}_p}{dt}=\boldsymbol{u}_p, \tag{1}$$

$$\frac{d\boldsymbol{u}_p}{dt}=\frac{g_1}{\tau_p}(\boldsymbol{u}-\boldsymbol{u}_p), \tag{2}$$

$$\frac{dT_p}{dt}=\frac{1}{m_p C_{\mathrm{coal}}}\left(A_p\alpha g_2(T-T_p)+A_p\varepsilon_p(G-\sigma T_p^4)\right)+\Delta h_{\mathrm{devol},k}\frac{dV_k}{dt}+Q_{\mathrm{char}}\frac{dC}{dt}, \tag{3}$$

$$\frac{dm_p}{dt}=-\sum_k\frac{dV_k}{dt}+\frac{dC}{dt}. \tag{4}$$

Here, τ_p is the particle relaxation time ($=\rho_p d_p^2/18\mu$, where ρ_p is the particle density and d_p is the particle diameter), C_{coal} the heat capacity of the coal particle, A_p the surface area of coal particle, α the heat transfer coefficient between the gas and dispersed-coal phases, σ the Stefan-Boltzman constant, ε_p the emissivity of particles, Q_{char} the heat source due to char combustion, C the mass of fixed carbon. $\Delta h_{\mathrm{devol},k}$ is the heat sink due to devolatilization and water evaporation and V_k the mass of chemical species k in volatile matter in coal. g_1 and g_2 are the correction coefficient of Stokes drag ($g_1=1+0.15Re_p^{0.687}$) [22] and the correction coefficient of heat transfer ($g_2=z/(e^z-1)$, $z=-C_p(dm_p/dt)/\pi d_p\lambda(2+0.552Re_p^{1/2}\mathrm{Pr}^{1/3})$) [23,24], respectively. For estimating ε_p and C_{coal}, the model of Baum and Street [25] is employed. G is the incident radiation flux and calculated by the discrete ordinate method (DOM)/S4 [26] with a coefficient of absorption obtained by the weighted sum of gray gases (WSGG) [27].

These equations are solved using an in-house thermal flow analysis code referred to as FK^3 (e.g., [11,12,28,29]). Interactions attributed to phase coupling between gas and dispersed-coal phases are calculated by a Particle-Source-In-Cell (PSI-Cell) model [30].

2.1. Mathematical models for coal particles

Heated coal particles yield char containing fixed carbon, nitrogen and ash, and volatile matter upon thermal decomposition. In previous DNS [20,21], the volatile matter is replaced by the methane, CH_4. However, in the present study, the devolatilization rate and compositions of the volatile matter of coal are obtained using the nitrogen and light gas (NLG) version of the chemical percolation devolatilization (CPD) model [31] to predict the amounts of light gases such as $CH_4, H_2O, CO_2, CO, H_2, C_2H_6, C_2H_4, C_3H_8$ and C_3H_6, and tar in the volatile matter. The compositions of $H_2, C_2H_6, C_2H_4, C_3H_8$ and C_3H_6 in the light gases and the tar are given under the following three assumptions [11]. First, a 0.4% mass fraction of H_2 in coal is generated. Secondary, light gases C_2H_6, C_2H_4, C_3H_8 and C_3H_6 are generated in mass fraction ratios of 1:1:0.5:1 in addition to CH_4, H_2O, CO_2, CO and H_2. Lastly, tar is composed of C_6H_6 (benzene). The first and second assumptions are based on the results of the pulverized coal pyrolysis experiment by Xu and Tomita [32]. In this study, the coal sample is Newlands [11], the properties of which are listed in Table 1. The compositions obtained based on the above assumptions are listed in Table 2. The devolatilization rate of volatile matter from coal particle is modeled as Arrhenius formulation proposed by Badzioch and Hawksley [33]. The fixed carbon in char begins to oxidize at the same time as the commencement of devolatilization. The change in the mass of the char associated with the oxidation reaction is estimated using the Field model [34].

Table 1
Properties of Newlands coal [11].

High heating value	29.1 MJ/kg
Low heating value	28.1 MJ/kg
Proximate analysis (wt.%)	
Moisture[a]	2.60
Ash[b]	15.20
Volatile matter[b]	26.90
Fixed carbon[b]	57.90
Ultimate analysis[b] (wt.%)	
Carbon	71.90
Hydrogen	4.40
Nitrogen	1.50
Oxygen	6.53
Combustible sulfur	0.39

[a] As received.
[b] Dry basis.

Table 2
Composition of volatile matter obtained using NLG version of CPD model [31].

Species	wt.%
H_2	0.84
H_2O	10.92
CO	6.37
CO_2	4.06
CH_4	9.68
C_2H_4	2.51
C_2H_6	2.51
C_3H_6	2.51
C_3H_8	1.25
C_6H_6	59.34

2.2. Computational details

The mono-dispersed pulverized coal particle-laden flow in a two-dimensional mixing layer is targeted. Fig. 1 shows the schematic diagrams of the computational domain and boundary conditions, and Table 3 shows the initial flow and coal particles conditions. The diameter of 25 μm, which is relatively smaller than that used in actual coal combustion furnaces, is chosen in order to enhance the devolatilization and to meet the requirement associate with the grid size from the point of view of numerical accuracy, respectively (the grid spacing needs to be roughly 10 times larger than the droplet size [35]). In order to enhance the ignition, coal particles in the central region of $-1.0\ \mathrm{mm} < y < 0\ \mathrm{mm}$ are initially heated up to 2000 K without giving any other heat sources. The reasons to employ this condition are that firstly, to avoid that shear vortices in the central region tended to achieve to the side boundaries before the ignition occurs. Secondary, according the fact that the coal particles are quickly heated up by radiation after injection in actual coal combustion furnaces, this condition is considered to be acceptable to understand the general behavior of ignition of coal particles. The dimensions of the computational domain are 30 mm and 30 mm in the streamwise and spanwise directions, respectively. The computational domain is divided into 300 (in x direction) and 350 (in y direction) computational grid points (uniform in x and clustered around $y \sim 0$ line in y direction). The grid