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Numerical investigation of the effects of volatile matter composition and chemical reaction mechanism on pulverized coal combustion characteristics



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ABSTRACT

Volatile matter is generally treated as postulated substance or a combination of different species because the detailed chemical compounds in volatile matter are not yet completely understood. However, very few studies investigate the effects of volatile matter composition and chemical reaction mechanism on the pulverized coal combustion characteristics. In this work, numerical simulations of pulverized coal laminar flames stabilized in a two-dimensional counterflow are conducted to examine these effects on the behaviors of pulverized coal combustion. The results show that the pulverized coal combustion characteristics can be changed considerably by slightly varying the species compositions in volatile matter. The pulverized coal flame structure calculated with large hydrocarbon volatile matter can be largely reproduced by a specific combination of light species. It is also shown that the pulverized coal flame structure cannot be correctly predicted by a single-step mechanism. Finally, it is found that both the stable thermo-chemical quantities and some intermediate species (e.g. OH) mass fractions are not sensitive to the choice of chemical reaction mechanism when detailed chemistry is considered.

1. Introduction

Numerical simulations have become an important tool to describe the characteristics of pulverized coal combustion [1–15] while experiments are extremely difficult to be conducted to provide such details [16]. Although significant progresses have been made in understanding the pulverized coal combustion characteristics, it is still very challenging to apply numerical simulations to practical pulverized coal combustors. The previous works were limited to simulate simplified laboratory scale flames [1,5,11,13]. However, the configurations and operating conditions of practical pulverized coal combustors are much more complicated, which cause additional difficulties in modelling studies. For example, biomass is often used in the co-firing pulverized coal combustion systems as a co-combustion fuel to reduce the emission of CO₂ [17–19]. Compared to pure pulverized coal combustion, numerical models for the co-firing of coal with biomass are difficult to be formulated due to the complicated raw material composition, the thermo-chemical structure of biomass, and the particle shape and motion, etc [18,19].

For pure pulverized coal combustion, four coupled steps are involved: (i) heating up/water evaporation, (ii) devolatilization, (iii) volatile matter combustion, and (iv) char surface reactions. The heating up/water evaporation process takes place as soon as the coal particles

are injected into the combustion system. This process does not involve reactions and can be accurately modelled. The subsequent devolatilization process is very important because it governs the coal particle ignition, combustion stability, pollutant formation and extinction [20]. Unfortunately, this process hasn't been well-characterized since the composition of volatile matter is not yet completely understood. In previous studies, the volatile matter is either treated as postulated substance C_xH_yO_z [4,11,10] or a combination of different species [1–3,5–9,12–14]. The species composition in volatile matter is usually determined empirically since the complete information is still not available from the experiment. For this reason, the volatile matter is often treated as different combinations of different species even for the same coal type [1,5,21]. For example, for the same Newlands bituminous coal [16], the volatile matter was treated as a combination of light gases such as CH₄, C₂H₂, CO, etc, in Refs. [1,5], while in Ref. [21], both light gases and larger hydrocarbons were included, in which the tar in volatile matter was assumed to be benzene (C₆H₆). However, the influences of the different treatments of volatile matter on the pulverized coal combustion characteristics have not been investigated yet. The third step of volatile matter combustion has been extensively investigated in recent years and significant progresses have been made [1,5–7,12,13]. The high-fidelity combustion models that are initially developed for gas combustion have been extended to pulverized coal

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combustion. Compared to previous studies with simplified gas combustion models [4,11,14,15], the predictions of species mass fractions and temperature have been improved with extended pulverized coal combustion models. For the final step of char surface reactions, the classical diffusion-kinetic-controlled surface reaction model developed by Baum and Street [22] was generally used in previous studies (e.g. Refs. [1–3,5–9,12–14]). The common assumptions are that devolatilization and char surface reactions occur sequentially and fixed carbon consists solely of carbon.

The selection of chemical reaction mechanism is another important aspect in pulverized coal combustion modelling studies. Depending on the species that are assumed for the volatile matter, different reaction mechanisms were utilized in previous studies. For example, single-step reaction mechanism was used in early studies to reduce the computational cost of direct numerical simulations [10,23] or the infinitely-fast chemistry gas combustion models were used [4,11]. In recent studies of high-fidelity gas combustion models [1,5,6,12,13], GRI-Mech 3.0 [24] and DRM-22 [25] were utilized when the volatile matter was treated as a combination of light gases. In more recent studies [21,9,7], more detailed kinetic mechanisms such as the CRECK mechanism [26] and the mechanism of Narayanaswamy et al. [27] were adopted where large hydrocarbons were available and the computational power is improved. The questions of interest include: what are the effects of chemical reaction mechanism on the pulverized coal combustion characteristics? Can simplified chemical reaction mechanisms characterize the main combustion behaviors of pulverized coal combustion?

In the above-mentioned context, the purpose of the present study is to investigate the effects of volatile matter composition and chemical reaction mechanism on pulverized coal combustion characteristics. To maintain a good balance between computational efficiency and accuracy, and to avoid the configuration-related complexity, the pulverized coal flames stabilized in a two-dimensional laminar counterflow are studied. According to the postulated volatile matter compositions, various chemical reaction mechanisms are evaluated, ranging from C1 to C6 chemical reaction mechanisms. The sensitivities of the volatiles and char mixture fractions, which are important trajectory variables in the flamelet model for pulverized coal combustion [1,2,5,6,12], to the studied parameters are evaluated in detail. In addition, various species mass fractions, including the minor species of OH and CH, calculated from different volatile matter compositions and chemical reaction mechanisms are also compared with each other. To the authors' best knowledge, it is the first study on the effects of volatile matter composition and chemical reaction mechanism on the pulverized coal combustion with finite rate chemistry combustion model.

The remainder of this paper is organized as follows. In Section 2, the numerical methods are presented. The computational setup and computational details are provided in Section 3. Results and discussion are given in Section 4. The last section provides a conclusion.

2. Numerical modelling

In the present work, the gas phase and solid phase are solved in Eulerian and Lagrangian manners, respectively. The governing equations for the gas phase and particle phase will be presented in this section. In addition, the two-way coupling terms and the coal combustion sub-models are also detailed.

2.1. Gas phase governing equations

For detailed chemistry simulations, the following governing equations of mass, momentum, enthalpy and species mass fractions for the gas phase are solved directly without averaging or filtering,

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = \dot{S}_{C,m} \quad (1)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2\mu}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right] + \dot{S}_{C,u_i} \quad (2)$$

$$\frac{\partial(\rho H_e)}{\partial t} + \frac{\partial(\rho u_j H_e)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho \alpha \frac{\partial H_e}{\partial x_j} \right) + \dot{S}_{C,H_e} \quad (3)$$

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_j Y_k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_k \frac{\partial Y_k}{\partial x_j} \right) + \dot{\omega}_k + \dot{S}_{C,m,k} \quad (4)$$

where u_i is the gaseous phase velocity, ρ is the gaseous phase density, which is calculated from the state equation for ideal gas, μ is the dynamic viscosity, p is the static pressure, δ_{ij} is the Dirac delta function, H_e is the specific total enthalpy, α is the thermal diffusion coefficient, Y_k is the mass fraction of species k , D_k is the mass diffusivity of species k , which is calculated under the assumption of unity Lewis number. $\dot{\omega}_k$ is the reaction rate of species k , which is calculated with different chemical reaction mechanisms according to the postulated volatile matter compositions, as described in the following context. $\dot{S}_{C,i}$ is the two-way coupling term, which will be given in Section 2.3.

2.2. Solid phase governing equations

Each coal particle is assumed to be composed of volatile matter, char and ash, and the little portion of water in the studied Newlands bituminous type coal [16] is added to the ash content by assuming dry coal particle. For simplicity, the ash is assumed as an inert substance, and the char is assumed to be only composed of carbon (i.e. C(s)), while the volatile matter is treated as different combinations of different species, which will be detailed in Section 2.4. Based on the above assumptions, the coal particle mass change can then be calculated as follows, describing the evolution of volatiles and char,

$$\frac{dm_p}{dt} = \frac{dm_{vol}}{dt} + \frac{dm_{char}}{dt} \quad (5)$$

where m_p , m_{vol} and m_{char} are the instantaneous mass of a single coal particle, volatile matter and char, respectively.

The motion of a single coal particle in gas–solid flows is described using Newton's second law. As the density of coal particles is much larger than that of the gas phase, only the drag and gravity forces are of importance. The motion equation for a coal particle can then be described as,

$$\frac{du_{p,i}}{dt} = \frac{3C_D \rho}{4d_p \rho_p} (u_i - u_{p,i}) u_{rel} + g_i \quad (6)$$

where $u_{p,i}$ is the coal particle velocity in the i th direction, d_p is the particle diameter, and ρ_p is the coal particle density. u_{rel} is the relative velocity between gas and particle, namely $u_{rel} = |\vec{u} - \vec{u}_p|$, C_D is the drag coefficient which is calculated using Wen-Yu's formulation [28], and g_i is the gravity acceleration in the i th direction.

Neglecting the Stefan flow effect [1,2,5], the particle energy evolution can be calculated as,

$$\frac{m_p C_{p,p} dT_p}{dt} = \frac{m_p C_{p,g} Nu}{3Pr} \left(\frac{T - T_p}{\tau_d} \right) + \dot{S}_{rad,p} + \dot{S}_r \quad (7)$$

where $C_{p,p}$ is the specific heat of coal particle, T and T_p are the gaseous and particle temperatures, respectively. Pr is the Prandtl number set to be 0.6 [29], Nu denotes the Nusselt number calculated by the Ranz-Marshall model [30], $Nu = 2 + 0.552 Re_p^{1/2} Pr^{1/3}$, where Re_p is the particle's slip Reynolds number. τ_d denotes the particle relaxation time defined as, $\tau_d = \rho_p d_p^2 / (18\mu)$. $\dot{S}_{rad,p}$ characterizes the radiative heat transfer between coal particle and gas phase, which will be presented in Section 2.4. \dot{S}_r is the temperature source term due to devolatilization and char-oxidation, which is calculated according to Ref. [15].

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