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Direct numerical simulation of a pulverized coal jet flame employing a global volatile matter reaction scheme based on detailed reaction mechanism

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ABSTRACT

A two-step global reaction scheme for the volatile matter of coal is proposed, and the unsteady coal particle and combustion behaviors in a turbulent pulverized coal jet flame are investigated by performing a direct numerical simulation (DNS) employing the proposed global reaction scheme. The two-step global reaction scheme is constructed to take into account the properties of the volatile matter such as transport coefficients, laminar flame speed and unburned gas temperature and to be applicable to various coal types, and it is validated by comparing the results with those obtained by the detailed reaction mechanism which includes 158 chemical species and 1,804 reactions. The validity of the DNS is also assessed by comparing the results with those in the previous experiment (Hwang et al., 2005) [16], and the unsteady coal particle motions and combustion characteristics are examined in detail. The results show that the proposed two-step global reaction scheme for the volatile matter of coal can precisely predict the laminar flame speed and burned gas temperature for various coal types from bituminous to low-rank coals over wide ranges of conditions of equivalence ratios, pressures and unburned gas temperatures. In addition, it can correctly take into account the effects of dilutions by H_2O and CO_2 which compromise the evaporated moisture from coal and products of char reaction. It is also verified that a lab-scale turbulent pulverized coal jet flame is well predicted by the DNS employing the proposed global reaction scheme. That is, the pulverized coal particles' velocity and its fluctuation and the characteristics of particle preferential motions are in general agreement with those observed in the experiment. The DNS reveals that in the turbulent pulverized coal jet flame, there appear premix and diffusion flame layers inside and outside, respectively. In addition, the reaction of the volatile matter and O_2 in coal-carrier air occurs in the inner premixed flame layer, whereas the reactions of the volatile matter and CO and O_2 in surrounding air occur in the outer diffusion flame layer.

1. Introduction

Coal occupies the position of a major primary energy source internationally because of its low procurement costs attributed to the large amount of recoverable reserves, widespread reserves, and stable supply. However, since 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 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.

Most coal-fired power plants employ pulverized coal combustion in which finely ground coal with particles several tens of micrometers in size is transported into the furnace with air and burned. 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 their surrounding air, release of flammable gases (volatile matter) from the particles, heterogeneous reactions, and gas-phase reactions, all of which are greatly affected by turbulence. Therefore, obtaining detailed information that cannot be measured (e.g., flow field, temperature field, concentration field, and the behavior of the pulverized coal particles) using numerical simulations is considered invaluable in designing and developing furnaces efficiently. As a calculation method for such information, a RANS (Reynolds-Averaged Navier–Stokes) simulation (e.g., [1–7]) to solve flow fields and scalar fields in an averaged time period and a LES (Large-Eddy Simulation) (e.g., [8–14]) to solve flow fields and scalar fields by taking only relatively large-scale turbulence fluctuations into account are being researched. A DNS (Direct Numerical Simulation), which does not use either a turbulence model or a

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turbulent–chemistry interaction model, can reproduce the effects of the turbulence on the above-mentioned elementary processes with greater accuracy than that achieved by the RANS simulation and LES, and DNS is expected to become a useful method for understanding the phenomenon of pulverized coal combustion in turbulence. However, researches employing DNS involve enormous calculation costs. Therefore, few studies have been conducted on virtual or simple pulverized coal flames (e.g., Luo et al. [15]), meaning that calculations employing the data of actual pulverized coal flames and detailed comparative reviews with the experimental data have not been conducted in any study. In fact, Luo et al. [15] performed a DNS of a pulverized coal flame referring to the experiment [16] targeted here. However, the calculation conditions such as initial gaseous temperature and Reynolds number, and coal characteristics in Luo et al. [15] are quite different from those in the experiment [16].

In order to conduct such numerical simulations on pulverized coal combustion, physical models are needed for the handling of the pulverized coal particles, and improving the accuracy of the model is a major challenge. In particular, the gas-phase reaction of volatile matter of coal is an extremely important elementary process that controls the behavior of pulverized coal combustion. However, the modeling of the reaction has not been discussed sufficiently. The reason for this lies in the facts that the volatile matter is a gas mixture consisting of light gases such as CH_4, CO, CO_2, and water vapor (H_2O) and tars, including aromatic compounds, and that the composition of these gases significantly differs depending on the type of coal [17]. This makes it difficult to apply a uniform reaction model. Previous researches often disregarded the effects of such complex compositions on the gas-phase reaction and instead used a model where the volatile matter was replaced with CH_4 (e.g., [7,8,15]). This is one of the reasons why the accuracy of predictions by the numerical simulations of pulverized coal combustion is compromised. For example, Stein et al. [11] conducted an LES for pulverized coal combustion and suggested that the reaction model used for the volatile matter was the cause behind the discrepancy between the predicted O_2 concentrations and measured values.

The purpose of this study is, therefore, to propose a precise global reaction scheme for the volatile matter of coal, and to investigate the coal particle and combustion behaviors in a turbulent pulverized coal jet flame by performing the DNS employing the proposed global reaction scheme. The global reaction scheme is constructed to take into account the properties of the complicated volatile matter such as transport coefficients, laminar flame speed and unburned gas temperature and to be applicable to various coal types. The validity of the DNS is assessed by comparing the results with those of the previous experiment [16], and the unsteady coal particle motions and combustion characteristics are examined in detail.

2. Global reaction scheme for volatile matter of coal

2.1. Construction procedure

Owing to the different molecular structures of the volatile matter of coals, their compositions differ with the coal types. Further, the volatile matter yield and its compositions strongly depend on the coal heating temperature and heating rate, because the release of the volatile matter is related to chemical reactions. Therefore, it is very difficult to identify the volatile matter yield and its compositions for each coal through experiments. In this study, the global reaction scheme for the volatile matter of coal is constructed in the following manner.

2.1.1. Determination of compositions based on ultimate analysis and proximate analysis

The devolatilization rate and compositions of the volatile matter of coal can be obtained using coal pyrolysis models such as CPD (Chemical Percolation Devolatilization) model [18], FG–DVC model [19] and FLASHCHAIN model [20]. In this study, the NLG (nitrogen and light gas species) version of CPD model [18] is used 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 assumptions:

(i) A 0.4% mass fraction of H_2 in coal is generated.
(ii) 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.
(iii) 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 [17]. The third assumption is employed because the calculation of the laminar flame speed based on the detailed reaction mechanism is limited to monocyclic aromatic hydrocarbons at present. It should be noted that the amount of H_2 strongly affects the combustion characteristics, and that the density of the volatile matter changes with the composition of tar. Therefore, these approximations need to be improved in future for more advanced calculations.

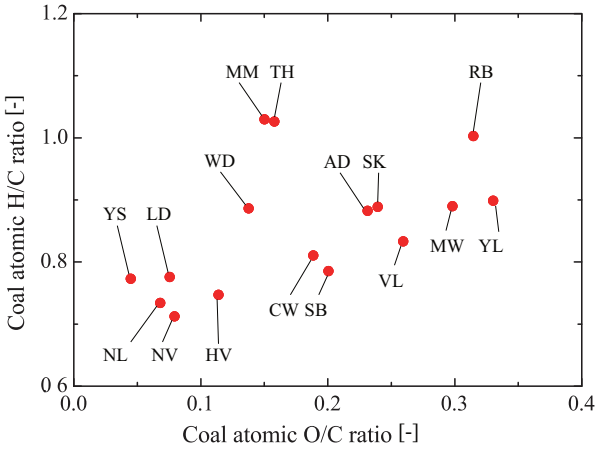

Fig. 1. Coal atomic H/C ratio versus coal atomic O/C ratio (van Krevelen diagram [21]).

In order to take into account the effect of the heating rates on the composition of the volatile matter, the numerical simulations of the pyrolysis of coal using the CPD model [18] are carried out for three coal heating rates: 1.0×10^4 K/s, 1.0×10^5 K/s and 1.0×10^6 K/s. The initial coal temperature and the pyrolysis maximum temperature are set to be 300 and 1300 K, respectively. The pyrolysis is found to finish at less than 1300 K in the CPD model, so that the pyrolysis maximum temperature is set to be 1300 K, here. In all, 16 types of coals are used; this includes 14 types of coals used by Xu and Tomita [17] and Newlands coal and Adaro coal. Their properties are listed in Table 1, and the relation of coal atomic H/C ratio and O/C ratio (van Krevelen diagram [21]) is also shown in Fig. 1. Here, Wandoan coal, Hunter Valley coal, Liddell coal, Newvale coal, Yubari Shinko coal, and Newlands coal are classified into bituminous coal, and the other coals are classified into low-rank coals such as sub-bituminous and brown coals. The input parameters for the CPD model [18] were obtained from the proximate and ultimate analysis through the correlation of Genetti et al. [22]

Figure 2 shows the effects of carbon content and heating rates on volatile matter yield for the 16 coals. Here, the carbon content is based on a dry-ash-free (daf) basis. Figure 3 also shows the effects of carbon content and heating rate on mass fractions of chemical species in volatile matter for the 16 coals. It is found that with increasing the carbon content, the volatile matter yield decreases, the hydrocarbon