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Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

Effect of multiphase radiation on coal combustion in a pulverized coal jet flame

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ARTICLE INFO

Article history:

Received 15 September 2016

Received in revised form

14 February 2017

Accepted 7 March 2017

Available online 15 March 2017

Keywords:

Coal radiation

Monte Carlo

Nongray

ABSTRACT

The accurate modeling of coal combustion requires detailed radiative heat transfer models for both gaseous combustion products and solid coal particles. A multiphase Monte Carlo ray tracing (MCRT) radiation solver is developed in this work to simulate a laboratory-scale pulverized coal flame. The MCRT solver considers radiative interactions between coal particles and three major combustion products (CO₂, H₂O, and CO). A line-by-line spectral database for the gas phase and a size-dependent nongray correlation for the solid phase are employed to account for the nongray effects. The flame structure is significantly altered by considering nongray radiation and the lift-off height of the flame increases by approximately 35%, compared to the simulation without radiation. Radiation is also found to affect the evolution of coal particles considerably as it takes over as the dominant mode of heat transfer for medium-to-large coal particles downstream of the flame. To investigate the respective effects of spectral models for the gas and solid phases, a Planck-mean-based gray gas model and a size-independent gray particle model are applied in a frozen-field analysis of a steady-state snapshot of the flame. The gray gas approximation considerably underestimates the radiative source terms for both the gas phase and the solid phase. The gray coal approximation also leads to under-prediction of the particle emission and absorption. However, the level of under-prediction is not as significant as that resulting from the employment of the gray gas model. Finally, the effect of the spectral property of ash on radiation is also investigated and found to be insignificant for the present target flame.

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1. Introduction

Thermal radiation plays a significant role in coal combustion, especially for the emerging new clean coal combustion technologies, such as oxy-coal combustion [1] and combined coal-magneto-hydrodynamics cycle [2]. There either the concentrations of CO₂ and H₂O are high or the overall temperature is elevated. To accelerate the development of such new technologies, an accurate and predictive coal radiation model is necessary. The modeling of radiation during coal combustion is first complicated by its multiphase nature: the particulate media including coal, char and fly ash, emit, absorb, and scatter with different spectral properties. Second, radiatively participative gaseous combustion products, mainly CO₂, H₂O, and CO have spectral properties that are very different from those of the particulate phases. The elevated CO₂ concentration in coal combustion,

especially in oxy-coal combustion, can alter the heat transfer pattern from convection-dominant to radiation-dominant [1]. The accumulation of H₂O in coal combustion with wet recycling enhances the possibility of radiation re-absorption as well. Third, unlike other multiphase fuel mixtures such as sprays, coal particles are active emitter due to the combination of high emissivity and high temperature. These aspects of thermal radiation in coal combustion, i.e., propagation of radiation through a particulate medium, the difference between participative gas phase and particulate phase radiative properties, and the emission and absorption by coal particles, have to be considered to accurately model and predict the heat transfer process in coal combustion.

Several radiation solvers, such as the P_N methods [3,4] and the discrete ordinates method [5] have previously been adopted to simulate the coal radiation for their computational expediency. The expensive but accurate Monte Carlo ray tracing (MCRT) method has been applied to combustion applications involving mainly gaseous media [6,7]. In the area of coal combustion, the MCRT method has been applied to solve the radiative transport equation (RTE) [8,9] only recently, due to the recent improvements in computing capabilities. Despite constraints such as high

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computational cost and long execution times, the MCRT method has the advantage of reproducing exact solution for sufficiently large statistical samples and the ability to treat inhomogeneous participative media and complex geometries with relative ease. This advantage is crucial for coal radiation modeling because coal combustion often involves both inhomogeneous participative media and complex geometries.

Besides an accurate solver for the RTE, the models for the spectral properties of the coal particles and the gas phase are also crucial for obtaining accurate radiation solutions. Simple gray models are commonly used for coal combustion [10,11]. However, coal, char, fly ash, and the gas phase have distinct spectral properties. Gray models, such as the constant-absorption-coefficient model and the weighted-sum-of-gray-gases model (WSGGM), cannot correctly predict the spectral properties of the mixture without *ad hoc* tuning. Recently, some detailed nongray spectral models are examined in the context of coal combustion [8,12]. Both the full spectrum *k*-distributions model [12] and the line-by-line (LBL) model [9] have been applied to account for the nongray gaseous properties of coal combustion. For coal particles, models that employ large particle limit assumptions [13], as well as the size-dependent Buckius-Hwang correlations [14] are examined in various coal combustion simulations [9,12,15]. To quantify the effects of radiative heat transfer in coal combustion, the present study attempts to bring together the most accurate RTE solver and the most accurate spectral models available for both the gaseous and particle phases. With the increasing computing power, the high-fidelity radiation models become less prohibitive. Therefore, it is a worthwhile exercise to bring the predictive power to the simulation of coal radiation.

The objective of this study is twofold: first, to develop a high-fidelity multiphase MCRT method that accounts for nongray properties of gas and particle phases and second, to investigate effects of nongray spectral properties through parametric studies using a laboratory-scale jet coal flame. In addition to the detailed radiation models, the developed coal combustion solver features a transient Reynolds-averaged Navier-Stokes-based (RANS) Eulerian-Lagrangian multiphase flow solver, a detailed gas-phase chemistry model and the potential of considering turbulence-chemistry-radiation interactions. The flow solver is expected to provide transient information on the number densities of coal particles with reasonable accuracy, which has been found to be essential in predicting the overall effects of radiation [4].

This article is organized as follows. The target flame is introduced in Section 2, followed by the description of the physical models and numerical methods in Section 3. In Section 4, results obtained using the proposed models are presented and discussed, and conclusions are drawn in Section 5.

2. The target flame

The target configuration is a laboratory-scale pulverized-coal jet flame. The flame was studied experimentally to investigate the ignition and pyrolysis characteristics of different coal types and coal feed rates [16]. Radiation effects for different size groups of coal particles, as well as lift-off heights and coal burnout rates, were measured in the experiments, for three coal jet flames with different stoichiometric ratios. Only the condition of a stoichiometric ratio of 0.22 is presented in this study where coal particles are injected through a central nozzle with a feed rate of 6.08 mg/s. The Reynolds number of the central jet is approximately 4400 based on the inlet air viscosity and velocity. Coal particles are ignited by a preheated gas mixture formed by catalytic combustion of propane that contains hot O₂, N₂, CO₂ and H₂O (Table 1). The hot coflow is injected through the square slit as indicated in Fig. 1. The proximate and ultimate analysis of the coal particles used in the experiments are listed in Table 2.

The target flame has been the subject of several modeling studies,

Table 1
Operating conditions.

| | Primary jet | Preheated mixture |
|------------------------|-------------|-------------------|
| Average velocity (m/s) | 10 | 4.8 |
| Temperature (K) | 300 | 1510 |
| Mass fraction (-) | | |
| N ₂ | 0.768 | 0.761 |
| O ₂ | 0.232 | 0.101 |
| CO ₂ | 0.0 | 0.093 |
| H ₂ O | 0.0 | 0.045 |

including both RANS- and large eddy simulation-based (LES) methods [11,15,17]. These simulations show reasonable agreements with the experimental data in some aspects, but also substantial differences in others. Each simulation has a different focal area, ranging from validating combustion models [15,17] to implementing accurate and inexpensive devolatilization model [11]. It has been postulated in the previous studies that the radiative heat flux is comparable to the convective heat flux after ignition and a better radiation model might improve the accuracy of the prediction of flame lift-off heights.

3. Models and methods

In this section, the models and solution methods are presented. Details on the RTE solver and spectral models will be discussed in Sections 3.1 and 3.2, respectively, followed by the descriptions of the turbulent multiphase combustion models in Section 3.3. The remaining numerical details are described in Section 3.4.

3.1. The RTE solver

A Monte Carlo ray tracing (MCRT) method is chosen to solve the RTE. The MCRT method can naturally account for the nongray effects of heterogeneous participative media, as well as isotropic/anisotropic scattering. With its stochastic nature, the MCRT method can be easily coupled with other stochastic models to capture turbulence-radiation interactions. Therefore, it is a suitable candidate because the nongray emission/absorption and scattering for the coal-gas mixture are of interest. Instead of directly solving the RTE mathematically, the MCRT method solves radiation transport by emitting and tracking a statistically large number of “energy rays” to account for their interaction with participating media. Each of these energy rays carries a specific amount of energy, and has a specific wavenumber, direction, and origin. They are emitted everywhere within the computational domain. The strength of each energy ray is proportional to the local emission potential of its host cell. The selection algorithms of the origin, propagation direction, and wavenumber of each energy ray are based on random number relations and have been reported in [6,13,18]. As each ray moves through the domain, it loses energy due to absorption by local participating media, and also scatters (i.e., changes direction) according to the scattering potential along its travel path. Each energy ray is tracked until its energy is completely absorbed by the participative media or it hits and/or exits the computational boundaries.

For the multiphase system, the total emission from participating media within the *i*th finite volume/cell, $Q_{emi,i}$, is equal to the sum of the emission from both the gas and solid phases. The quantity is calculated as

$$Q_{emi,i} = Q_{emi,g,i} + Q_{emi,s,i}, \quad (1)$$

where the subscripts *g*, *i* and *s*, *i* represent gas and solid phases in cell *i*, respectively. $Q_{emi,g,i}$ and $Q_{emi,s,i}$ are the emission from gas and

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