Combustion and Flame 161 (2014) 1866–1882

Contents lists available at ScienceDirect

Combustion and Flame

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

Transported PDF modeling of pulverized coal jet flames

Xin-Yu Zhao *, Daniel C. Haworth

Department of Mechanical and Nuclear Engineering, The Pennsylvania State University, University Park, PA 16802, United States

ARTICLE INFO

Article history:
Received 28 October 2013
Received in revised form 17 December 2013
Accepted 19 December 2013
Available online 24 January 2014

Keywords:
Pulverized coal flames
Coal combustion modeling
Probability density function method

ABSTRACT

A transported composition probability density function (PDF) method is developed for pulverized coal combustion. A consistent hybrid Lagrangian particle/Eulerian mesh algorithm is used to solve the modeled PDF transport equation for the gas phase, with finite-rate gas-phase chemistry. The model includes k–ε turbulence, gradient transport for scalars, and a Euclidean minimum spanning tree (EMST) mixing model. A separate Lagrangian description is used to solve for the coal particle phase, including particle tracking, coal devolatilization and surface reaction models. Interphase coupling models are developed to handle the interaction between the gas phase and the solid phase. Radiative heat transfer is modeled by a $P1$ model for a gray absorbing emitting and scattering gas–particle system. Two independent laboratory-scale pulverized coal jet flames ("flame A" and "flame B") are simulated using the new model. For flame A, the baseline model reproduces the measured mean and rms particle axial velocity reasonably well. Some discrepancies are found in particle temperature and gas-phase concentrations, which may in part be due to the uncertainties in the experimental data. Sensitivities of model results to coal-related model variations, turbulence–chemistry interactions, different interphase coupling strategies, and finite-rate chemistry are explored to establish sensitivities and to determine which aspects of the models are most important. The same model is applied to a second flame (flame B), the only change being in parameters related to the different coal composition. It is found that experimental standoff heights cannot be reproduced for three different stoichiometric ratios using a single model. Time scales for chemical reactions, devolatilization and turbulence are extracted and compared, to study the level of turbulence–chemistry–particle interactions in flame A and to test the popular assumption of equilibrium chemistry in coal combustion modeling. Mixture-fraction statistics for flame B are explored to test assumptions that have been proposed for mixture-fraction-based coal models. While the usual assumption of Beta distributions is found to be appropriate, assumptions of statistical independence of two mixture fractions are not valid.

1. Introduction

Coal combustion is, and is expected to remain, a major source of electricity generation, especially for countries including the United States and China that have high electricity demand and large coal reserves [1]. Recent research interest on coal focuses on increasing combustion efficiency while decreasing pollutant and greenhouse-gas emissions, such as NOx and CO_2. Among the various possible ways of efficiency enhancement and CO_2 reduction, direct power extraction using magnetohydrodynamics (MHD) combined with high-temperature oxy–coal combustion has been revisited recently [2]. High-fidelity computational fluid dynamics (CFD) models are desired to help design and optimize the combustion systems, due to the scarcity of experimental data and lack of experience in these high-temperature environments, where furnace temperature can be as high as 3000 K, with high concentrations of radicals, CO_2 and H_2O.

The process of pulverized coal combustion can be divided into four main steps: heating up/water evaporation, devolatilization, volatile gases combustion, and char surface reactions. Accurate property data and physical submodels are required for quantitative predictions [3–6]; these include the thermodynamic properties of coal components, devolatilization rates and components, surface reaction rates, coal off-gas mixing and combustion, and interactions between particles, turbulence, chemistry and radiation.

Turbulence–chemistry interactions (TCI) is one aspect that has received little attention to date. Turbulence–chemistry interactions can be important in determining the correct mixing level for volatile gases evolved from the particle phase. Under rapid heating conditions, variations in devolatilization and surface-reaction rates due to turbulent fluctuations are another manifestation of turbulence–chemistry interactions. In most of the turbulent coal combustion modeling studies, simple models such as the eddy-breakup (EBU) model and eddy-dissipation-concept (EDC) model

* Corresponding author.
E-mail addresses: xzz105@psu.edu, zhaoxy02@gmail.com (X.-Y. Zhao).

0010-2180/$ - see front matter © 2013 The Combustion Institute. Published by Elsevier Inc. All rights reserved.
http://dx.doi.org/10.1016/j.combustflame.2013.12.024

have been used to account for the effect of turbulence–chemistry interactions [6]. These models are not expected to be as accurate as higher-fidelity models, such as the conditional moment closure (CMC) model [7] and transported probability density function (PDF) models [8]. Models that have been designed specifically for turbulent coal combustion can have different limitations; for example, the widely used local equilibrium chemistry assumption cannot capture the effects of finite-rate chemistry (e.g., CO oxidation) [9]. As large-scale computational power has become more widely available, more research efforts have focused on incorporating higher-fidelity models that have been developed for gaseous turbulent flames, into coal combustion modeling [10–12]. For example, a comprehensive set of coal combustion models, including a transported velocity-composition PDF model for the gas phase, has been established in [11]. One limitation of the method developed in [11] is the adoption of local equilibrium chemistry, which might not be sufficient if the prediction of slowly reacting species such as CO is desired, because CO concentrations can be significantly above equilibrium values in pulverized coal flames [5]. An important aspect of the modeling effort in dual-Lagrangian-particle formulations such as that used in [11] (coal particles and gas-phase notional particles) is the interaction between phases, as represented through modeling of the interphase source terms [10,11].

The purpose of this research is to develop a comprehensive model for high-temperature pulverized coal combustion, such as that encountered in the combustor for an open-cycle MHD system, with particular emphasis on the turbulence–chemistry interaction models. This is being pursued by coupling a transported composition PDF method with realistic finite-rate gas-phase chemical mechanisms and widely-employed coal submodels. A systematic approach is being pursued for model development. In earlier work, simulations were performed for laboratory syngas–air nonpremixed flames [13] and a high-temperature oxy-natural gas system [14]. There the models were extended towards the thermochemical environments of interest, without the complications of coal particles, and good agreement with experiment was realized. The next step is to add coal particles and coal combustion, and that is the subject of this paper. In the earlier work, a stochastic Lagrangian particle method was used to implement the transported PDF method, including realistic finite-rate chemistry. Here a separate Lagrangian description is adopted for the solid phase (coal particles).

Compared to the mixture-fraction-based models that have been employed earlier in coal simulations, the use of a detailed composition specification here in terms of species mass fractions and mixture specific enthalpy allows one to handle situations such as multiple inlets with different compositions (e.g., natural gas–coal co-firing) and non-adiabatic systems in a more natural manner. Without additional effort on the gas-phase modeling, it can also accommodate different evolution rates of different coal off-gas components, if the devolatilization model provides information on individual mass evolution rates. And finite-rate chemistry, such as CO oxidation, can also be captured, by properly choosing the gas-phase chemical mechanism.

In this paper, the framework for extending a transported composition PDF method to coal combustion is established first. The reliability of existing PDF submodels (e.g., mixing models) and numerical strategies (e.g., ISAT [15]), is explored, in this complicated new environment. Model results are compared with experimental measurements for two different pulverized coal–air flames. Variations in key models and model parameters are then made to explore the sensitivities. Finally, the high-fidelity model is used to test key assumptions that have been made in simpler mixture-fraction-based models for turbulent coal combustion.

The rest of the paper is organized as follows. In the following section, the target flames are introduced and findings from earlier modeling studies are summarized. In Section 3, the numerical methods and physical models are described. Comparisons with experimental measurements and sensitivities to variations in models are reported in Section 4. Finally, key findings are summarized and next steps are outlined.

2. Pulverized-coal jet flames

A laboratory-scale methane-piloted pulverized-coal jet flame is the first target configuration, and will be referred to as "flame A" (Table 1). The flame was studied experimentally at the Japanese Central Research Institute of Electric Power Industry (CRIEPI) [16]. As a laboratory-scale jet flame, coal particles are injected through a central nozzle, carried by air. The main jet is surrounded by a methane annular jet, which is ignited first, and serves as a pilot to ignite the coal particles. The Reynolds number of the central jet flow is approximately 2500 based on ambient viscosity, which is transitional rather than fully turbulent. Measurements reported in [16] include axial mean and rms particle velocities, axial mean particle temperature, radial distributions of coal particle size at different axial locations, and mean mole fractions of O_2, CO_2, CO and N_2. Compared to global parameters such as carbon burnout and ignition delay, these detailed measurements more fully reveal the structure of the jet coal flame. Newland bituminous coal was used in the experiments; the composition of the coal particles and the heating values are listed in Table 2. The injected particle-size distribution is also given in [16]. The boundary conditions for this flame are thus reasonably well defined, compared to other available data sets. Figure 1 shows the geometry of the injector.

Flame A has been the subject of several modeling studies, using both RANS- and LES-based methods [17–20]. Bermudez et al. [17] used this flame to validate their group combustion models. There volatile gases were assumed to burn infinitely fast on a flame front. A basic assumption of the group combustion model is that no oxygen is left inside the flame zone, while no volatile fuel is present outside the flame. Judging by the experimental oxygen measurements, this assumption might not be valid for this flame. Hashimoto et al. [19] implemented a tabulated devolatilization model (TDP model), which can account for the influence of varying heating rates on the devolatilization rates. Comparisons were made between the TDP model and conventional single-rate and two-rates models. By carefully choosing the model parameters, the conventional models could give results similar to those from the TDP model. However, these parameters are case-dependent and require a priori knowledge of the heating condition of the system, so that the TDP model is more predictive. In [18,20], three research groups used different LES-based coal combustion codes to explore the same flame, and differences of the results from the different models were used to draw conclusions regarding which aspects of the modeling were most important. It was postulated that a better turbulence–chemistry-interaction model might improve the oxygen prediction along the centerline.

All the available studies showed reasonable agreement with the experimental data in at least some respects. The largest disagreements were seen in the gas-phase concentrations and solid-phase temperature. However, arguments have also been made concerning the reliability of the experimental data, especially for the

Table 1
Inlet specifications for flame A.

Coal feed rate	1.49×10^{-4} kg/s
Air flow rate	1.80×10^{-4} m^3/s
Methane flow rate	2.33×10^{-5} m^3/s