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Prediction of oxy-coal flame stand-off using high-fidelity thermochemical models and the one-dimensional turbulence model

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Abstract

An Eulerian one-dimensional turbulence (ODT) model is applied to simulate oxy-coal combustion, with specific aim at predicting flame stand-off distances. Detailed gas-phase chemical kinetics based on the GRI3.0 mechanism are utilized. A high-fidelity model for devolatilization is considered that predicts evolution of several light gas species as well as char as products of devolatilization. The mass, momentum and energy governing equations are fully coupled between the particle and the gas phase. Likewise, char oxidation and gasification are both considered. Results indicate that char oxidation and gasification are both significant during the later stages of devolatilization. The impact of radiative temperature and mixing rate on oxy-coal flame is simulated and discussed where flame stand-off is used as a metric to compare the simulation prediction with experimental data. The data show evidence that there is kinetic limitation to the flame standoff distance. Finally, results show that ODT can provide quantitative agreement with experimental data in predicting flame standoff in oxy-coal jet flames.

Keywords: One-dimensional turbulence; Turbulent combustion; Coal combustion; Oxy-coal combustion; Devolatilization

1. Introduction

Among the promising technologies to capture CO_2 for subsequent sequestration in new and existing coal-fired power plants is oxy-coal combustion. In the process of oxy-coal combustion, oxygen mixed with recycled flue gas is used as an oxidizer rather than air. Models to predict the physics of such a system must address the nonlinearly coupled processes of particle dynamics, gas-phase thermochemistry, heterogeneous reactions between the coal and gas, devolatilization/pyrolysis, vaporization, radiative heat transfer, etc. This multiscale (in both space and time) problem poses a significant modeling challenge.

Models for coal devolatilization vary widely in complexity. Arrhenius-form models such as single-rate [2] and Kobayashi [17] models are among the relatively simple models that describe devolatilization with a kinetic rate. The distributed activation energy model [1] uses a gaussian distribution for the activation energy. Among the more

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complex models, chemical percolation devolatilization (CPD) considers thermal decomposition of the macromolecular network and accounts for structural variation in coal types [3,9,33]. In a more advanced version of the CPD model, rate equations corresponding to various light gas species are utilized in order to predict the light gas composition [14], providing an opportunity to couple directly with detailed chemistry in the gas phase.

Numerous studies on oxy-coal combustion and gasification physics, in particular the ignition delay, flame stability and temperature, flame shape, impacts of oxygen and diluent have been undertaken (see, *e.g.*, [5,10,12,13,20,24]). Various experiments have measured the impact of coal type and operating conditions such as composition of coal transport medium on flame stand-off and stability [27,39].

Applying direct numerical simulation (DNS) with detailed gas-phase kinetics and coal devolatilization models can help improve understanding of ignition and can provide a basis for evaluating simpler models. However, it remains prohibitively expensive to perform DNS in regimes relevant to practical coal combustion. In this work, an Eulerian formulation of the one-dimensional turbulence (ODT) model is used. ODT resolves the full range of length and time scales of the continuum (as in DNS) but in a single spatial dimension, thereby significantly decreasing the computational cost relative to DNS. First proposed by Kerstein [16], ODT has been successfully applied to a variety of turbulent flows, including particle-laden flows [30] and turbulence-chemistry interaction including extinction and reignition [18,26]. Most notable among the assumptions in ODT is that the flow field is statistically one-dimensional (implications of this assumption are discussed in [25,35]). In this work, ODT is used to simulate oxy-coal flames and is evaluated against experimental data [28,39].

The aim of this work is to assess the effects of system parameters as well as model parameters on the prediction of flame stand-off distance in a 40 kW coal combustor [27,28], and to demonstrate the efficacy of the ODT model in modeling turbulent coal combustion. The impact of the "eddy rate constant" (which affects the mixing rate in ODT), radiative temperature, and primary O_2 concentration on the flame stand-off is explored. This is the first work of its kind that determines flame stand-off distance using detailed kinetic calculation of the gas phase fully coupled to a high-fidelity model (CPD) for devolatilization of coal particles.

2. Governing equations

The equations governing gas and particle (coal) phases are summarized in this section.

2.1. Gas phase

An Eulerian formulation of ODT [35] adapted to solve multiphase reacting flows is applied in this work. The conservation equations are

$$\frac{\partial \rho}{\partial t} = -\frac{\partial v}{\partial y} + S_{\mathrm{p}m}, \tag{1}$$

$$\frac{\partial \rho v}{\partial t} = -\frac{\partial \rho v v}{\partial y} - \frac{\partial \tau_{yy}}{\partial y} - \frac{\partial P}{\partial y} + S_{\mathrm{p}v}, \tag{2}$$

$$\frac{\partial \rho u}{\partial t} = -\frac{\partial \rho v u}{\partial y} - \frac{\partial \tau_{yx}}{\partial y} + S_{\mathrm{p}u}, \tag{3}$$

$$\frac{\partial \rho e_0}{\partial t} = -\frac{\partial \rho e_0 v}{\partial y} - \frac{\partial p v}{\partial y} - \frac{\partial \tau_{yy} v}{\partial y} - \frac{\partial q}{\partial y} + S_{\mathrm{p}e_0}, \tag{4}$$

$$\frac{\partial \rho Y_i}{\partial t} = -\frac{\partial \rho Y_i v}{\partial y} - \frac{\partial J_i}{\partial y} + \omega_i + S_{\mathrm{p}Y_i}, \tag{5}$$

where u and v refer to streamwise and spanwise velocities, respectively, mixture-averaged approximations are used for diffusive fluxes, and P is obtained via the ideal gas equation of state. $S_{\mathrm{p}m}$, $S_{\mathrm{p}v}, S_{\mathrm{p}u}, S_{\mathrm{p}e_0}$ and $S_{\mathrm{p}Y_i}$ are interphase exchange terms for mass, y-momentum, x-momentum, total internal energy and species respectively (see Section 2.3) and the p subscript denotes a particle-phase property. Here, the y-direction is taken as the spanwise direction. A reduced GRI mechanism consisting of 24 species and 86 reactions [32] is utilized for the gas-phase kinetics treatment. Transport equations are solved for the species, with appropriate phase-exchange source terms for the devolatilization, vaporization, and char oxidation processes occurring on particles.

2.2. Particle phase governing equations

Newton's second law is employed to describe the motion of each particle

$$m_{\mathrm{p}} \frac{\mathrm{d}u_{\mathrm{i,p}}}{\mathrm{d}t} = m_{\mathrm{p}} g_{\mathrm{i}} + S_{\mathrm{p},v} + F_{\mathrm{p}}, \tag{6}$$

where i denotes the i^{th} direction, m_{p}, $u_{i,\mathrm{p}}, g_{\mathrm{i}}, S_{\mathrm{p}_j,v}$, and F_{p} are mass of single particle, particle velocity, gravity acceleration, force generated by fluid-particle interaction, and force generated by particle–particle interaction. For this study, particle–particle interaction is neglected ($F_{\mathrm{p}} = 0$) and the drag force is described by Stokes' law so that the particle momentum equations become

$$\frac{\mathrm{d}\vec{u}_{\mathrm{p_j}}}{\mathrm{d}t} = \frac{\vec{g}_i\left(\rho_{\mathrm{p}} - \rho_{\mathrm{g}}\right)}{\rho_{\mathrm{p}}} + S_{\mathrm{p},\vec{u}}, \tag{7}$$

where $(S_{\mathrm{p_j},\vec{u}})$ is given by Eq. (11) in Section 2.3. The position of the jth particle in the ith direction (x_{i,p_j}) is determined by

$$\frac{\mathrm{d}x_{i,\mathrm{p_j}}}{\mathrm{d}t} = u_{i,\mathrm{p_j}}. \tag{8}$$