



A comparative study of thermochemistry models for oxy-coal combustion simulation



Babak Goshayeshi*, James C. Sutherland

The University of Utah, Department of Chemical Engineering, Unites States

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ABSTRACT

In this work, the One-Dimensional Turbulence (ODT) model is used to evaluate various thermochemistry models for capturing flame stand-off distance in oxy-coal combustion. In the gas phase, calculations made with detailed chemical kinetics are compared with results using an infinitely-fast (flame-sheet) chemistry model. Models for vaporization, devolatilization and char oxidation/gasification are incorporated for each La-grangian coal particle. Two coal devolatilization models, namely a simple two-step Arrhenius and Chemical Percolation Devolatilization (CPD), are compared. The governing equations (mass, momentum and energy) are fully coupled between the particle and the gas phase. Flame stand-off distance determined by the simulation is compared with experimental results. Results show that the flame stand-off distance predicted by the infinitely-fast chemistry model is shorter than the prediction obtained by the detailed chemical kinetics model and that flame stand-off distance using two-step model is longer than the CPD model. Furthermore, it was observed that the minimum flame stand-off distance is determined by the devolatilization model and does not show sensitivity to the gas phase model. However, the shape of flame stand-off PDF is significantly altered by changing the gas-phase kinetic model.

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1. Introduction

Oxy-coal combustion is one of the promising options for CO₂ capture in coal-fired furnaces. Numerical simulation of oxy-coal combustion can improve knowledge of this process and improve design to further increase efficiency while also decreasing greenhouse gas emissions. In this work, different levels of modeling in the gas (carrier) and coal particle (dispersed) phases are compared and analyzed.

The devolatilization process has a considerable impact on the ignition delay of coal particles, and models for devolatilization vary widely in terms of complexity and formulation. The single-rate [1] and two-step [2] models describe the devolatilization model using one and two Arrhenius-form kinetic rate(s), respectively. The Distributed Activation Energy (DAE) model attempts to account for changes in the structure of coal during devolatilization [3]. These simpler models produce nondescript volatile gas-phase species. Network models treat the devolatilization process as a breakdown of macromolecular networks to produce gas-phase species [4]. Among network models, the Chemical Percolation Devolatilization (CPD) model treats coal as a macromolecular network of aromatic rings that are connected with bridges [5,6]. Jupudi et al. [7] proposed a more ad-

vanced version of the CPD model that determines the yield of light gas species over the course of devolatilization and is the most advanced devolatilization model considered in this work.

Gas-phase kinetics are frequently treated in a simplified form, relying on the existence of low-dimensional manifolds to describe chemistry by reduced-order models such as flame-sheet, equilibrium, flamelet, etc. The flame-sheet model describes the gas phase reactions by a single, infinitely fast, one-step irreversible reaction, and is among the simplest descriptions of gas-phase chemistry and implies a mixing-limited description of chemistry. Using the “mixed-is-burned” assumption and also accounting for molecular dissociation in the gas phase, the equilibrium model is also a common approach [8,9]. In a further advancement, the flamelet model relaxes the infinitely fast chemistry assumption by describing the degree of departure from the equilibrium state using the scalar dissipation rate. The flame-sheet and flamelet models have been applied to simulate ignition of single coal particles [10,11]. In each of these cases, a turbulent closure is typically also included to describe the unresolved fluctuations in composition [12]. Another commonly used model for chemistry modeling in turbulent flow is the Eddy Dissipation Concept (EDC). This model (along with the detailed devolatilization model) has been applied to coal combustion/gasification by Vascellari et al. [13,14].

In any modeling approach, a trade-off between computational cost and fidelity/accuracy is made. This work investigates the impact

* Corresponding author.

E-mail address: b.goshayeshi@gmail.com (B. Goshayeshi).

of a range of models for both devolatilization and gas-phase chemistry on simulation predictions. Models on both ends of the spectrum of cost/fidelity are compared to experimental data for flame stand-off distance in an oxy-coal system.

To resolve the full range of length and time scales of the continuum as in direct numerical simulation, but at a significantly lower computational cost, Kerstein [15] proposed the One-Dimensional Turbulence (ODT) model. ODT resolves the full range of length and time scales, but in a single direction and the effects of turbulent mixing are modeled. A Eulerian formulation of ODT model that solves evolution of velocity and scalars along a one-dimensional line of sight in a three-dimensional turbulent flow field is applied in this work [16,17]. The capabilities of the ODT model have been previously established for particle-laden flows [18] and turbulence-chemistry interaction (including extinction and reignition) [19,20] and oxy-coal combustion [21].

Previous ODT simulations of a 40 kW oxy-coal combustor [22–24] have examined the impact of system and model parameters on flame stand-off [21]. In [21], detailed gas phase kinetics were paired with the CPD devolatilization model. Previous work by the authors has also considered the effect of particle size, environment temperature and coal type for laminar, single-particle scenarios [10]. The aim of this work is to study the impact of chemistry models in coal and gas phases on prediction of flame stand-off. Specifically, we consider pairings of two devolatilization models (CPD and two-step) with two gas-phase chemistry models (detailed kinetics and flame-sheet). The choice of these models covers relatively simple (two-step devolatilization and flame-sheet gas-phase chemistry) to high-fidelity (CPD and detailed gas kinetics) and provides some insight into the effect of model fidelity on flame stand-off predictions.

2. Model formulation

2.1. Conservation equations

The governing equations for mass, momentum, energy and species for the gas and the particle phase are presented here. More detail can be found in [17],[10],[16],[21], and [25].

2.1.1. Gas phase

In the gas phase, conservation equations are solved for mass, momentum¹ and energy:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial v}{\partial y} + S_{pm}, \quad (1)$$

$$\frac{\partial \rho v}{\partial t} = -\frac{\partial \rho v v}{\partial y} - \frac{\partial \tau_{yy}}{\partial y} - \frac{\partial P}{\partial y} + S_{pv}, \quad (2)$$

$$\frac{\partial \rho u}{\partial t} = -\frac{\partial \rho v u}{\partial y} - \frac{\partial \tau_{yx}}{\partial y} + S_{pu}, \quad (3)$$

$$\frac{\partial \rho e_0}{\partial t} = -\frac{\partial \rho e_0 v}{\partial y} - \frac{\partial p v}{\partial y} - \frac{\partial \tau_{yy} v}{\partial y} - \frac{\partial q}{\partial y} + S_{pe_0}, \quad (4)$$

$$\frac{\partial \rho Y_i}{\partial t} = -\frac{\partial \rho Y_i v}{\partial y} - \frac{\partial J_i}{\partial y} + \omega_i + S_{pY_i}, \quad (5)$$

where ρ is the density, v and u are velocity components in the x and y directions, e_0 is the total energy and Y_i is the mass fraction of species i . Source terms appearing in the above equations will be defined in Section 2.4. Eqs. (1)–(5) are completed by the ideal gas

equation of state, $P = \rho RT/M$ and constitutive relationships for the diffusive fluxes

$$\tau_{yy} = -\frac{4}{3}\mu\frac{\partial v}{\partial y}, \quad (6)$$

$$\tau_{yx} = -\mu\frac{\partial u}{\partial y}, \quad (7)$$

$$q = -\kappa\frac{\partial T}{\partial y} + \sum_{i=1}^{n_s} h_i J_i, \quad (8)$$

$$J_i = -\frac{\rho Y_i}{X_i} D_i^{mix} \frac{\partial X_i}{\partial y}, \quad (9)$$

where μ and κ are viscosity thermal conductivity; h_i , X_i and D_i^{mix} are the species enthalpy, mole fraction and mixture-averaged diffusivity, respectively. S_{pm} , S_{pv} , S_{pu} , S_{pe_0} and S_{pY_i} are particle source terms for mass, y and x velocities, energy and species, respectively, that are described in [10],[21], and [25]. Finally, the gas phase temperature is determined from the internal energy, composition and pressure via a newton-solve. In the ODT, stochastic eddy events representing turbulent mixing are modeled in a manner that has been shown to reproduce salient statistics including the $\frac{5}{3}$ energy cascade [15] as well as extinction and reignition in combusting flows [19].

2.1.2. Particle phase

On each particle, conservation equations are written for mass, velocity and temperature:

$$\frac{dm_p}{dt} = \frac{dm_{H_2O}}{dt} + \frac{dm_v}{dt} + \frac{dm_c}{dt}, \quad (10)$$

$$\frac{du_p}{dt} = \frac{g_x(\rho_p - \rho_g)}{\rho_p} + S_{p,u}, \quad (11)$$

$$\frac{dv_p}{dt} = \frac{g_y(\rho_p - \rho_g)}{\rho_p} + S_{p,v}, \quad (12)$$

$$\frac{dT_p}{dt} = \frac{-A_p}{m_p C_p} [h(T_p - T_g) + \epsilon \iota (T_p^4 - T_r^4)] + S_{p,T}, \quad (13)$$

where m_{H_2O} , m_v , m_c are the mass of moisture, volatile and char in the coal particle and m_p is the total mass of particle, u_p and v_p are velocities of particle at x and y directions, respectively. T_p , T_g and T_r are particle, gas and effective radiative temperatures, respectively. A_p , C_p and ρ_p are particle surface area, heat capacity and density respectively. The convective heat transfer coefficient is represented by h ; also, ϵ and ι are the emission coefficient and Stefan–Boltzmann constant, respectively. Source terms appearing in the above equations will be defined in Section 2.4.

Additional equations for the composition of each particle are solved depending on the models chosen for vaporization, devolatilization and char oxidation/gasification.

The particle diameters are constant during the simulation and mass conservation Eq. 10 affects the particle density. Inter-particle interaction and particle swelling are not considered.

2.2. Gas phase chemistry

Two different gas-phase chemistry models are considered in this work: detailed kinetics and infinitely fast (flame-sheet) chemistry. In both models, the species transport is fully coupled with the particle transport. A brief description of these models is given below, with additional details provided in [10].

2.2.1. Detailed chemistry

To address detailed chemistry in the gas phase, a reduced GRI3.0 mechanism consisting of 24 species and 86 reactions is utilized [26]. This mechanism has also been applied in the previous study [21]. The

¹ Only two components of momentum are solved here: the component parallel to the ODT direction and the primary streamwise component. See [16] and [17] for more information.

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