



# A comparison of various models in predicting ignition delay in single-particle coal combustion



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## ABSTRACT

In this paper, individual coal particle combustion under laminar conditions is simulated using models with various levels of complexity for the particle and gas phase chemical kinetics. The mass, momentum and energy governing equations are fully coupled between the particle and the gas phase. In the gas phase, detailed chemical kinetics based on GRI3.0 and infinitely-fast chemistry are considered and compared. For the particle phase, models for vaporization, devolatilization and char oxidation/gasification are considered, and the Kobayashi–Sarojim devolatilization model is compared to the Chemical Percolation Devolatilization (CPD) model. Ignition delay is used as a quantitative metric to compare the simulation prediction with experimental data, with careful attention given to the definition of ignition delay in the simulations. The effects of particle size, coal type and gas-phase temperature on the ignition delay are studied and compared with experimental data.

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## 1. Introduction

Coal combustion/gasification is a complex process with many coupled sub-processes occurring simultaneously [1]. Furthermore, most practical coal combustion systems are turbulent, further complicating the modeling challenge because of the nonlinear coupling occurring across a multitude of length and time scales. Even with modern day computers, resolving the entire physics of the problem remains prohibitively expensive. Coal combustion/gasification models must address particle dynamics in turbulent flow, gas-phase thermochemistry, heterogeneous reactions between the coal and gas, devolatilization/pyrolysis, vaporization, radiative heat transfer, etc.

The modeling challenge for coal combustion is further complicated by the varying properties and chemical structure of different coal types [2], and by the fact that the coal properties change significantly throughout a coal particle's lifetime in a combustor [3–5]. The coal particle thermochemistry in this work is divided into three processes: vaporization, devolatilization and char oxidation/gasification.

Models for devolatilization vary widely in complexity, with the most sophisticated models accounting for the chemical structure of the coal and its effect on the devolatilization process [1]. In 1971, a constant value was proposed for the combustion rate of each coal type [6]. Arrhenius-form models such as the single-rate [7] and Kobayashi [8] models describe devolatilization with a kinetic rate.

In 1976, the Distributed Activation Energy (DAE) model [9] proposed using a Gaussian distribution for the activation energy. Determining the parameters for the Gaussian distribution were the challenges of this model [10]. Representing coal as a collection of functional group including aromatic rings, aliphatic chains and bridges and oxygen-carrying groups was a significant step in devolatilization modeling [11,12]. The Chemical Percolation Devolatilization (CPD) model accounts for the thermal decomposition of the macromolecular network and accounts for structural variation among various coal types [13,14,1], and can accurately describe light-gas evolution from coal devolatilization [15]. In this work, the Kobayashi and CPD devolatilization models (representing a relatively simple and fairly sophisticated model, respectively) are utilized; their ability to predict ignition delay are examined.

Char oxidation and gasification are heterogeneous reactions, and are significantly slower than the vaporization and devolatilization processes [1,16]. There are many factors influence the char oxidation, such as coal structure, coal type, the gas-phase environment (e.g., oxygen partial pressure) and temperature [17,18]. The products of char oxidation are mainly carbon dioxide and monoxide [19,20]. A common assumption in coal combustion modeling is that char oxidation occurs after the coal particle is fully devolatilized [21,22]. The present study and formulation allow for simultaneous vaporization, devolatilization and char oxidation and do not impose any temporal ordering/sequencing of these processes.

The influence of systems parameters such as oxidizer composition and coal rank on ignition delay and flame stability have been explored experimentally by several researchers [23–29]. A review on experiments measuring the coal particle ignition delay is

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reported in [30]. In [25], the influence of gas phase temperature and particle size on the single particle ignition delay are also considered as parameters. In this work, the ignition delay is employed as metric to evaluate simulation results where the effect of gas phase temperature, coal rank and particle size on ignition delay are studied and compared to the experiments conducted by [25].

Although numerous simulations of coal combustion have been performed, most use relatively simple models for the devolatilization and gas-phase combustion process [31–35]. The flamelet and flame-sheet models are used in simulation of single coal particle combustion by different groups [36,34,31]. Attempts to address limitations of these models have used two- and four-step global mechanisms [26]. Hecht et al. performed one-dimensional simulations on char oxidation of single coal particles with detailed kinetics to determine the temperature and species radial profiles for char oxidation, but used boundary-layer assumptions to treat diffusion [37–39].

The objective of this work is to evaluate the efficacy of devolatilization and gas-phase chemistry models for coal combustion/gasification. To this end, we compare experimental observations of coal particle ignition delay to two devolatilization models paired with two gas-phase kinetics models. To the authors' knowledge, this is the first computational study examining ignition delay using detailed kinetics in the gas phase fully coupled to a high-fidelity model (CPD) for devolatilization of coal particles. We consider the effect of key parameters including particle size, furnace temperature, and coal type on the ignition delay time, and evaluate a few simplified modeling strategies relative to the detailed models and experimental data.

This paper is organized as follows: the governing equations are described in Section 2. Section 3 then provides a description of the models for gas-phase kinetics and coal particles (including evaporation, devolatilization, char oxidation/gasification). The simulation results, including trends with varying the reactor temperature and particle sizes, are discussed in Section 5, and compared to experimental ignition delay data.

## 2. Governing equations

The governing equations for gas and particle phase are provided in this section. A one-dimensional domain aligned with the  $y$ -coordinate that evolves in time was considered in this work.

### 2.1. Gas phase

The gas-phase equations are solved in an Eulerian frame of reference. The overall mass conservation equation in the gas phase is

$$\frac{\partial \rho}{\partial t} = -\frac{\partial v}{\partial y} + \sum_{j=1}^{n_p} S_{pjm}, \quad (1)$$

where  $\rho$  is the gas phase density,  $v$  is the gas velocity at  $y$  direction (lateral),  $S_{pjm}$  is the particle source term accounting for interphase mass exchange and  $n_p$  is the total number of particles (in this work, simulations are performed for a single particle). Individual species conservation equations accounting for interphase mass exchange are given as

$$\frac{\partial \rho Y_i}{\partial t} = -\frac{\partial \rho Y_i v}{\partial y} - \frac{\partial J_i}{\partial y} + \omega_i + \sum_{j=1}^{n_p} S_{pjY_i}, \quad (2)$$

where  $Y_i$ ,  $J_i$  and  $\omega_i$  are the mass fraction, mass-diffusive flux and reaction source term of species  $i$ , respectively, and  $S_{pjY_i}$  is the release rate of species  $i$  from particle  $j$  into the gas phase.

Momentum equations are evolved for the component of momentum aligned with the resolved ( $y$ ) direction and one orthogonal component,

$$\frac{\partial \rho v}{\partial t} = -\frac{\partial \rho v v}{\partial y} - \frac{\partial \tau_{yy}}{\partial y} - \frac{\partial P}{\partial y} + \sum_{j=1}^{n_p} S_{pjv}, \quad (3)$$

$$\frac{\partial \rho u}{\partial t} = -\frac{\partial \rho v u}{\partial y} - \frac{\partial \tau_{yx}}{\partial y} + \sum_{j=1}^{n_p} S_{pju}, \quad (4)$$

where  $v$  and  $u$  refer to lateral and streamwise velocities, respectively. Finally, the energy equation is

$$\frac{\partial \rho e_0}{\partial t} = -\frac{\partial \rho e_0 v}{\partial y} - \frac{\partial p v}{\partial y} - \frac{\partial \tau_{yy} v}{\partial y} - \frac{\partial q}{\partial y} + \sum_{j=1}^{n_p} S_{pje_0}, \quad (5)$$

where  $e_0$  is the internal energy and  $q$  is the heat diffusive flux. Closure of this system is achieved by the ideal gas equation of state,  $P = \rho RT/M$  and constitutive relationships for the diffusive fluxes [40]

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

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

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

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

where  $\mu$  is the viscosity,  $\kappa$  is the thermal conductivity,  $h_i$  is the species enthalpy,  $X_i$  is a species mole fraction,  $D_i^{\text{mix}}$  is the species mixture-averaged diffusivity and  $n_s$  is the number of species. Here,  $\mu$ ,  $\kappa$  and  $D_i^{\text{mix}}$  are functions of temperature, pressure and composition. Finally, temperature is obtained from the internal energy via a Newton-solve that incorporates the variation in composition and pressure.

The source terms  $S_{pm}$ ,  $S_{pv}$ ,  $S_{pu}$ ,  $S_{pe_0}$  and  $S_{pY_i}$ , which account for interphase heat, mass and momentum transfer, will be described in Section 2.3. Corresponding exchange terms are included in the particle phase governing equations.

Additional models can be incorporated to include the effects of turbulent mixing [41,40]. For the purposes of this paper, only laminar flow is considered to isolate the effects of the thermochemical models from the turbulence models. Further discussion and derivation of the gas-phase governing equations can be found in [40,42].

### 2.2. Particle phase

Particles are transported in a Lagrangian frame of reference where each particle's position, velocity, mass, and thermochemical state are evolved. Although they have mass and volume, it is assumed that the particles do not displace fluid on the Eulerian mesh where the gas-phase equations are solved. Rather, particle source terms are interpolated onto the mesh and gas-phase quantities are interpolated to the particle location for purposes of interphase coupling. This assumption is reasonable provided that the gas phase mesh spacing is large relative to the particle size, which is the case for the simulations performed here. The motion of a single particle in gas–solid flows can be described by using Newton's second law

$$m_p \frac{du_{i,p}}{dt} = m_p g_i + S_{pj,v} + F_c, \quad (10)$$

where  $i$  denotes the  $i$ th direction,  $m_p$ ,  $u_{i,p}$ ,  $g_i$ ,  $S_{pj,v}$ , and  $F_c$  are mass of single particle, particle velocity, gravity acceleration in  $i$ th direction, force generated by fluid–particle interaction, and force

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