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Full Length Article

An evaluation of the efficacy of various coal combustion models for predicting char burnout

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HIGHLIGHTS

- Evaluation of several coal combustion models with varying levels of fidelity.
- Effect of varying environmental parameters on burnout calculations investigated.
- Significant overlap in devolatilization and char oxidation is predicted.

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ABSTRACT

Coal combustion is comprised of several subprocesses including devolatilization and heterogeneous reactions of the coal char with O_2, CO_2, H_2O and potentially several other species. Much effort has been put forth to develop models for these processes which vary widely in both complexity and computational cost. This work investigates the efficacy of models for devolatilization and char reactions at either end of the complexity and cost spectrums for a range of particle sizes and furnace temperatures and across coal types. The overlap of simulated devolatilization and char consumption is also examined. In the gas phase, a detailed kinetics model based on a reduced version of the GRI 3.0 mechanism is used. The Char Conversion Kinetics and an n^{th}-order Langmuir-Hinshelwood models are considered for char oxidation. The Chemical Percolation and Devolatilization and a two-step model are considered for devolatilization. Results indicate that high-fidelity models perform better at representing particle temperature and mass data across a wide range of O_2 concentrations as well as coal types. A significant overlap in devolatilization and char consumption is observed for both char chemistry and devolatilization models.

1. Introduction

Coal combustion is a complex process that involves a number of highly-coupled physical phenomena, including reaction and transport of gas phase species, exchange of material between the gas and particle phases, and in many cases, the presence of turbulent flow. Modeling these processes, and their nonlinear interactions, in industrial-scale coal boilers poses a significant challenge. It is common practice to use empirical models for coal subprocesses in place of those with greater complexity [1–4], and even determine the beginning or end of some phenomena such as char oxidation *a priori* in order to reduce the computational load of performing needed calculations [2]. Furthermore, large variations in parameters such as particle diameter, furnace temperature, and oxygen concentration may occur within a single furnace. Therefore, it is important to know what effect these parameters have on quantities-of-interest such as particle mass and temperature over a range of model complexities, especially in the realm of char oxidation, which occurs over a much greater time span than evaporation and devolatilization.

Much effort has been put forth in development of char reaction models spanning a range of complexity. The simplest models use Arrhenius expressions that rely only on the partial pressure of species in the vicinity of the particle [1] and employ a global approach to the char reaction kinetics, while some go a step further and require calculation of surface partial pressures [5,6]. Yet more detailed models endeavor to resolve the physical subprocesses that occur during char oxidation and gasification. CBK-type models based on work by Hurt et al. [7], such as the CBK-E [8], and CBK-G [9] model char reaction kinetics based on the physical characteristics of the coal, and often include various submodels for evolution of particle diameter, char reactivity, and formation of an ash film. Possibly the most advanced CBK-type model is the Char Conversion Kinetics (CCK) model developed by Shurtz and Fletcher [10,11], which combines the gasification and oxidation kinetics of

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[9,8] and considers Stefan flow. The most advanced approaches go as far as to discretize the char particle into concentric shells [12] or discrete cubical elements [13] in order to fully resolve intraparticle species transport and kinetics.

Some recent work has examined the efficacy of various char reaction models over a range of input parameters and simplifying assumptions. Maloney et al. [14] compare particle density and diameter calculations from the CBK model in 6 and 12 mol% oxygen environments, and compare predictions to experimental observations. It was concluded that the CBK model generally does a good job at predicting trends in particle diameter and density and that accurate input data on distributions of initial size and density are required for obtaining good predictions. Gonzalo-Tirado et al. [15] consider several approaches to modeling CO oxidation around burning char particles of various sizes. They conclude that use of a single film model yields acceptable error in temperature and mass calculations for particles with diameters less than 200 μm and that the choice of gas phase chemistry model significantly impacts the calculated particle temperature. Work by Goshayeshi and Sutherland [16] investigates the performance of various combinations of gas phase chemistry and coal devolatilization models over a range of furnace temperatures and particle diameters for laminar, single particle combustion, but focuses on ignition rather than char oxidation/gasification. It appears that there is a very limited body of work that explicitly addresses the potential overlap in devolatilization and oxidation physics and its effect on char burnout predictions. Work by Biagini and Tognotti [17] examine the reactivities of chars from various fuel sources and found that char reactivity is enhanced when devolatilization and char oxidation are allowed to occur simultaneously rather than strictly sequentially. McConnell and Sutherland [18] examine the importance of model fidelity in particle and gas phase chemistry models on char burnout calculations, and demonstrate that the choice of gas phase model has a substantial effect on particle temperature calculations and less so on predicted char burnout. Devolatilization kinetics were found to have an impact on char burnout calculations, but overlap of devolatilization and char oxidation was not explicitly addressed. It appears that only [10,11,19,18] publish particle temperature or mass calculations using CCK, and of these only [18] considers char oxidation. In two other studies, CCK is used only to estimate the effect of CO inhibition on CO_2 gasification of petroleum coke [20] and biochar [21].

The purpose of this study is to investigate the efficacy of two char reaction models: the CCK model which takes an intrinsic approach to modeling oxidation, and the n^{th}-order Langmuir-Hinshelwood model which uses a global rate expression. The effect of varying furnace temperature and initial particle diameter on calculations using either the CCK or LH models is examined. Calculated particle heating rates due to convection, heterogeneous reaction, and radiation are investigated. Additionally, the effect of devolatilization on particle temperature and mass calculations is investigated by employing two separate devolatilization models in tandem with CCK and LH models. To the authors' knowledge, this work is the first to analyze, in-depth, the effect of varying furnace temperature and particle diameter on char burnout calculations while spatially resolving gas-phase transport and kinetics and implementing high-fidelity models for homogeneous kinetics, devolatilization, and char consumption.

2. Theoretical formulation

2.1. Gas phase

The gas phase conservation equations are written in an Eulerian reference frame as [16,22]

$$\frac{\partial \rho\phi}{\partial t} = -\frac{\partial \rho\phi u}{\partial x} - \frac{\partial \Theta_\phi}{\partial x} + \omega_\phi + \sum_{j=1}^{n_p} \frac{S_{p_j\phi}}{V_{\text{cell}}}, \tag{1}$$

where ϕ is an intensive quantity, Θ_ϕ is the diffusive flux of ϕ, ω_ϕ is the net rate of production of ϕ in the gas phase, V_{cell} is the quantity representing the volume of the control volume, and $S_{p_j\phi}$ is gas-phase source term for ϕ from the particle phase. In this formulation, $\phi = \{1, u, v, e_0, Y_i\}$ where ρ is the mass density, u and v are the x and y components of velocity, respectively, e_0 is the specific total internal energy, and Y_i are species mass fractions. For the continuity equation, $\phi = 1$ and $\Theta_\rho = 0$.

2.2. Particle phase

Particle transport is accomplished using a Lagrangian frame of reference where position, velocity, diameter, temperature, mass, and composition are time-evolved for each particle. Two way coupling of particle velocity, composition, and temperature with the gas phase is considered. Gas displacement by the particle is neglected. Details of the formulation are available in [16,22].

2.3. Interphase coupling

Source terms for each species are calculated by summing contributions from evaporation, devolatilization, reactions with char. Evaporation and devolatilization terms are described in [16], while char reaction models are discussed in Sections 2.5.1 and 2.5.2.

The energy evolved due to char oxidation is determined by

$$\Delta H^{\text{Ox}} = \frac{\varphi \Delta H^{\text{Ox}}_{CO_2} + \Delta H^{\text{Ox}}_{CO}}{1+\varphi}, \tag{2}$$

where φ is the instantaneous ratio of CO_2 to CO produced through char oxidation. The source term in the particle energy balance is given as

$$S_r = \frac{1-\alpha}{m_p C_p}\left[\Delta H^{\text{Evap}}\left(\frac{\mathrm{d}m_p}{\mathrm{d}t}\right)^{\text{Evap}} + \Delta H^{\text{Ox}}\left(\frac{\mathrm{d}m_c}{\mathrm{d}t}\right)^{\text{Ox}} + \sum_k \Delta H^{\text{G}}_k \left(\frac{\mathrm{d}m_c}{\mathrm{d}t}\right)^{\text{G}}_k\right], \tag{3}$$

where m_p and m_c are the particle and char masses, respectively, and $k = \{CO_2, H_2O, H_2\}$. Superscripts "Evap," "Ox" and "G" denote evaporation, oxidation, and gasification, respectively. Enthalpies of reactions used for heterogeneous reactions with char have values $H^{\text{Ox}}_{CO_2} = -3.308 \times 10^4$, $H^{\text{Ox}}_{CO} = -9.630 \times 10^3$, $H^{\text{G}}_{CO_2} = 1.437 \times 10^4$, $H^{\text{G}}_{H_2O} = 1.094 \times 10^4$, and $H^{\text{G}}_{H_2} = -6.234 \times 10^3$ kJ/kg. The parameter α is the fraction of energy evolved from heterogeneous reactions that is transferred to the gas phase. In previous studies [16,22,18], we have used $\alpha = 0.3$ based on work by Gu et al. [23]. However, as mentioned in [18], a constant value for α does not yield accurate particle temperatures over a wide range of conditions. The authors recently proposed a model for α as [24]

$$\alpha = \frac{h_p r}{\kappa_p + h_p r}, \tag{4}$$

where $\kappa_p = D^{\text{T}}_p \rho_p C_p$ is the particle thermal conductivity, D^{T}_p and ρ_p are the particle thermal diffusivity and density, respectively. h_p is the convective heat transfer coefficient [16], and r is the particle radius. Eq. (4) attempts to model the competing effects of intraparticle and interphase energy transfer among the hot products of char combustion in the immediate (unresolved) vicinity of the particle, the gas phase, and the particle. Intraparticle and interphase heat transfer are represented by κ_p and $h_p r$, respectively.