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Full Length Article

Resolved simulations of single char particle combustion in a laminar flow field

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HIGHLIGHTS

- Combustion of single char particles in a flow field is investigated with spatially and chemically resolved simulations.
- The mass and energy exchanges between the solid particle and the gas phase during combustion under oxy-atmosphere are studied comprehensively and compared with the corresponding cases in air.
- The impact of the particle flow motion on the flame that forms around the char particle is investigated by varying relative Reynolds number with particle size and relative slip velocity.

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ABSTRACT

The aim of this work is to study spatially and chemically resolved particle combustion cases to understand chemical and laminar transport processes and to support model development. In the present study, the combustion process of a single char particle located in air or oxy-fuel atmosphere composed of oxygen, carbon dioxide, and steam is investigated. Char burnout is represented in highly resolved numerical simulations including a detailed description of the surface and the gas phase chemistry. At the solid-gas interface, heat and mass fluxes due to the surface reactions involving carbon oxidation and gasification are considered. The model is validated based on experimental results for char burnout phase in a flat flame burner. We perform a comprehensive set of fully resolved reactive 2-D simulations by varying particle size, relative velocity, diluent, and oxygen composition in the surrounding gas. The simulation results are discussed regarding the CO_2 and N_2 content of the atmosphere highlighting the effects of oxy-fuel combustion. Furthermore, the impact of the particle flow motion on the flame that forms around the char particle is investigated by varying relative Reynolds number with particle size and relative slip velocity.

1. Introduction

Increasing carbon dioxide (CO_2) emissions in the atmosphere and its relation to global warming have become a great concern for the future of life on earth. Fossil-fuel-fired power plants, especially those burning coal, are among the main CO_2 emitters. Although the use of renewable energy sources is continuously growing, in the foreseeable future fossil fuels are still the major energy source due to their abundance and low price. Among fossil fuels, coal is one of the cheapest and the most available. To reduce CO_2 emissions from coal-fired power plants, CO_2 capture and storage techniques can be applied. Oxy-fuel combustion is one possible approach to recover CO_2. In oxy-coal fired furnaces, coal particles are burned in a mixture of oxygen and recycled flue gas (mainly CO_2) instead of burning in air (mainly N_2) typical for conventional burners [1]. In order to optimize oxy-coal fired burners, the understanding of the underlying physical processes is essential. A comprehensive review of several experimental and numerical studies that have been made to investigate oxy-fuel combustion of pulverized coal can be found in Chen et al. [2]. In the present study, numerical simulations are performed to investigate combustion of char particles, which remain in coal combustion after the so-called devolatilization process [3]. Both, air and oxy-fuel atmospheres are considered.

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Char possesses a porous structure and its main compound is carbon. Mass and energy transfer between a char particle and its surrounding gas can be modeled either by point particle or resolved particle approaches. Point particle models are typically used for practical applications on the large scale. In the resolved particle model, solid-gas interface and particle boundary layer are resolved chemically and spatially. Simulations based on the resolved particle model can describe interactions between chemistry and transport that can be used to understand the interaction of chemical and transport processes and to develop accurate models for application in large scale simulations using the point particle assumption. Several resolved simulations of char particle combustion have been described in the literature.

Maffei et al. [4] studied coal particle temperature and burnout time during combustion in air and oxy-fuel atmospheres by performing experiments and numerical simulation. Hecht et al. [5,6] simulated quiescent char combustion in N_2 and CO_2 diluents using a 1-D steady state model in SKIPPY (Surface Kinetics in Porous Particles). SKIPPY solves mass, momentum, and energy conservation for a reacting porous spherical particle and its reactive boundary layer. They studied the impact of CO_2 and steam gasification reactions on coal char combustion under oxy-fuel condition varying the O_2 concentration. Applying the same model, Shaddix et al. [7] performed numerical assessment of the CO_2/CO production ratio correlation presented by Tognotti et al. [8]. Furthermore, Hecht et al. [9] quantified errors associated with the two simplified common coal char combustion sub-models: the single film model originally proposed by Nusselt [10] and the double film model proposed by Burke and Schumann [11]. Their study was based on the 1-D steady state model and thus did not capture the char combustion history or interactions between flow and chemistry. Kestel et al. [12] and Richter et al. [13] performed steady 2-D simulations of char particle combustion in the flow of air and oxy-atmosphere, respectively. Richter et al. [13] compared 2-D simulations of spherical 200 μm particles to measurements carried out by Bejarano and Levendis [14]. They have investigated the influence of the relative Reynolds number, Re_{rel} of the char particle on its combustion behavior and observed that increasing Re_{rel} leads to higher carbon consumption rates. Although their model resolved the particle boundary layer spatially, chemistry was described based on a global mechanism. Furthermore, due to the steady state assumption in their model, the evolution of char combustion was not considered. Cho et al. [15] have successfully applied a 1-D model to study the evolution of liquid droplets and carbon particle combustion. Based on this transient-resolved model, further investigations on char combustion characteristics have been performed in Lee et al. [16,17]. Furthermore, Lee et al. [18] extended this transient-resolved model to a 2-D simulation and showed that finite Damköhler number effects can only be evident when detailed transport and chemical kinetics are included. Their study included char oxidation only in air atmosphere.

In the current study, a method similar to that of Lee et al. [18] is applied and validated by experimental measurement of particle temperature. Direct measurements of particle properties (temperature, diameter and even shape) have been subject to several studies in the past. These studies were carried out in laminar flow reactors, which provide well defined combustion atmospheres, representing air or oxy-fuel conditions. The gas phase temperature in these systems is provided from a gas flame, based on non-premixed (Hencken type [19–28]) or premixed (McKenna type [21,29–31]) combustion, or heated reactor walls [4,14,32–36]. For temperature measurements, different approaches were used, non-imaging techniques based on photomultipliers [4,14,19–22,25,26,32–36] deriving (equivalent spherical) particle diameter from intensities in different wavelength ranges [19–22,25,26,35,36] or preselected from previous sieve classifications of particle sizes [4,14,32–36] as well as imaging techniques [21,23,24,27,31] which derive particle diameter and additional 2-D projections [21] or 3-D [37,38] shape of burning char particles from the extend of the particle in the image simultaneous to the temperature measurement.

Temperature-diameter measurements have a significant advantage in particle combustion model development. There are at least two different applications of the measured data. First, rate law parameters for heterogeneous char consumption can be derived. This has been done for oxy-fuel char combustion using reaction rate models with varying complexity, e.g. in [19,24,27]. Second, such experimental data are useful for validation of the modeling results [4,24,39–42].

Here, 2-D resolved transient simulations of char combustion not only in air, but also under oxy-atmospheres are presented and discussed. Simulation results for both atmospheres are validated with experiments presented in more detail below. The reasons behind the different combustion behavior in air and oxy-atmosphere are analyzed and discussed. The interaction between chemistry and flow field is investigated in two parts. The first part demonstrates differences between cases with the same Re_{rel}, but varying particle size and relative velocity. In the second part, by varying the relative velocity, Re_{rel} is varied in the expected Re_{rel} interval for pulverized char particles in a swirl burner. The same set of simulations is performed for various oxygen concentrations (24%, 30%, and 36%). These simulations determine the influence of a relative flow on the carbon consumption rate and the heat released from char particle combustion.

2. Method

In the current study, combustion of a single particle in a laminar flow reactor is investigated. Fig. 1 shows a schematic view of the single particle located at 60 mm height of the burner. Combustion of the particle with diameter D_p is computed in a rectangular numerical domain, $[x_1^-, x_1^+] \times [x_2^-, x_2^+] = [-50D_p, 100D_p] \times [-50D_p, 50D_p]$ (see Fig. 1). The computational domain origin is set to the center of the particle. The computational domain was chosen large enough so that the particle combustion is not influenced by the domain boundaries. The particle is assumed to have fixed diameter and location. A mixture of gaseous species with a relative velocity with respect to the particle, U_1^0, enters the domain through the inlet at x_1^- and leaves the domain at x_1^+. To model solid particle combustion with surrounding gas flow, the conservation equations were solved in the solution domain consisting of gas, solid, and the interface between them.

2.1. Governing equations in the gas phase

Conservation of mass, species, momentum, and energy in the gas phase within the low-Mach formulation leads to the governing equations as [43]

$$\frac{\partial \rho_g}{\partial t} + \frac{\partial}{\partial x_\beta}(\rho_g U_\beta) = 0, \tag{1}$$

$$\frac{\partial \rho_g Y_i}{\partial t} + \frac{\partial}{\partial x_\beta}(\rho_g (U_\beta + V_{\beta,i}) Y_i) = \dot{M}_i, \tag{2}$$

$$\frac{\partial \rho_g U_\alpha}{\partial t} + \frac{\partial}{\partial x_\beta}(\rho_g U_\alpha U_\beta) = -\frac{\partial \Pi}{\partial x_\alpha} + \frac{\partial \tau_{\alpha\beta}}{\partial x_\beta}, \tag{3}$$

$$c_{p,g}\frac{\partial \rho_g T_g}{\partial t} + c_{p,g}\frac{\partial}{\partial x_\beta}\left(\rho_g U_\beta T_g\right) = \frac{\partial}{\partial x_\beta}\left(\lambda_g \frac{\partial T_g}{\partial x_\beta}\right) - \rho_g \times \frac{\partial T_g}{\partial x_\beta}\sum_i^n c_{p,i} Y_i V_{\beta,i} + \dot{Q}, \tag{4}$$