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### Numerical investigation and modeling of reacting gas-solid flows in the presence of clusters



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#### HIGHLIGHTS

• Clusters delay the conversion process by up to 85% compared to a homogeneous flow.

• The PDF of particle-phase volume fraction resembles a lognormal distribution.

• A 0D model that solves the temporal evolution of reactant mass fraction is derived.

• A presumed-shape PDF models the effects of clusters on reactant mass fraction.

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#### ABSTRACT

This work presents a volume-filtered formulation for describing chemically reacting flows in the presence of solid catalytic particles. The equations are discretized in a Eulerian-Lagrangian framework and applied to flows of isothermal, heterogeneously reacting chemical species in fully developed threedimensional risers. The aim of this study is to identify and quantify the influence of particle clusters on heterogenous reactions. The Archimedes number, Ar, is varied from 500 to 12,500, and the Damköhler number, Da, from 0.1 to 10. To assess the multiphase dynamic effects on the chemistry, conversion times from the three-dimensional simulations are compared to a zero-dimensional model that solves for the temporal evolution of the species mass fraction and ignores all spatial variations. The conversion process associated with the three-dimensional simulations is shown to be significantly longer compared to the zero-dimensional solution, with an increasing effect for larger values of Da. The discrepancies can be fully attributed to the presence of clusters, which are accounted for in the zero-order equations by an additional term that contains the covariance between species mass fraction and particle volume fraction fluctuations, which needs to be modeled. To this purpose, contributions to the fluctuating chemical source term are evaluated from the three-dimensional data and discussed, and a presumed-shape probability distribution function (PDF) approach is investigated. This PDF approach models the fluctuating chemical source term by a product of a beta distribution for the species mass fraction and a lognormal distribution for the particle concentration, and yields a mean species solution that agrees very well with the three-dimensional results for the range of Ar and Da considered in this study.

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#### 1. Introduction

Reactive gas-solid flows play a major role in a wide variety of engineering devices. Within the energy sector, such flows are used in fluidized bed reactors due to their low pressure drops, uniform temperature distribution, and high efficiency in mixing. Since the 1970s, circulating fluidized bed (CFB) reactors have been used in a range of technical processes, including fluid catalytic cracking (FCC)

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http://dx.doi.org/10.1016/j.ces.2014.10.005 0009-2509/© 2014 Elsevier Ltd. All rights reserved. (Avidan et al., 1990; Avidan, 1996), gasification and combustion of coal (Brereton, 1996; Lee, 1996; Basu, 2006), and more recently thermochemical conversion of biomass (Li et al., 2004; Sanz and Corella, 2006). Currently, catalytic-like processes (e.g., FCC) remain the primary conversion technique within the petrochemical industry (Speight, 2014), and is the focus of this study. A common feature of all reactive gas-solid systems is the complex processes occurring at the particle scale, referred heretofore as microscale processes. These include heat and mass transfer between the two phases, adsorption on and desorption from the solid surfaces, and the actual chemical reaction between the adsorbed gas and the solid (Szekely et al., 1976). If the variations in particle concentration becomes significant, the multiphase dynamics might impact the microscale processes significantly and therefore cannot be ignored. Within the riser of a CFB reactor, solid particles are pneumatically conveyed by a carrier gas phase, characterized by velocities much higher than minimum fluidization. The high flow rates encountered in risers often lead to the spontaneous generation of densely packed particles, referred to as clusters. Clusters have been observed to reduce mixing and interaction of particles with the transport gas (Shaffer et al., 2013), and therefore may inhibit the chemical conversion process, potentially lowering operating efficiencies significantly. Simultaneously accounting for both the microscale processes and particle dynamics poses significant challenges in developing predictive models. As a result, detailed studies demonstrating the quantitative impact of particle clustering on chemical processes occurring in such flows are severely limited.

Due to the importance of reactive gas-solid flows in industrial units and the large impact clusters have on operation efficiency, there exists great need for improved models that account for the presence of clusters during the design process. To this end, we wish to perform high fidelity simulations with the ultimate goal of extracting information that can be used to develop a predictive reduced-order model. In general, simulating chemical processes in fluidized bed reactors requires a chemical kinetic model to describe the various reactions taking place and a framework for solving gas-solid flows. In the context of catalytic cracking in risers, most work found in the literature models the solid phase as a continuous Eulerian field, greatly reducing the computational cost as individual particles do not need to be tracked (see e.g., Theologos and Markatos, 1993; Derouin et al., 1997; Treece et al., 1999; Gupta and Subba Rao, 2001; Das et al., ; Souza et al., 2006; Wu et al., 2008; Prasad Vegendla et al., 2012). In the limit where the flow is highly collisional and assumed to be nearly at equilibrium, the particle density function is close to Maxwellian and a Chapman-Enskog expansion can be used to derive a two-fluid model (TFM) using ensemble or volume averaging (Gidaspow, 1994; Zhang and Prosperetti, 1994; Peirano and Leckner, 1998). However, due to the strong coupling between the gas phase and solid particles, the solid concentration becomes highly segregated and the velocity distribution deviates far from equilibrium. Agrawal et al. (2001) demonstrated that global statistics obtained from Eulerian-Eulerian simulations of nonreactive riser reactors were strongly dependent on the mesh size but became mesh-independent when mesh size is of the order of a few particle diameters. As a result, accurate predictions obtained from TFM are potentially still excessively expensive for such flows. In a recent study, Ozel et al. (2013) employed TFM at various resolutions to obtain mesh-independent results in non-reactive CFB reactors. It was shown that various sub-grid terms have to be modeled in order to account for the unresolved clustering dynamics.

Eulerian-Lagrangian strategies provide an alternative framework that typically relies on simpler closures, where individual particle trajectories are solved using Newton's laws of motion, and models are required for interphase exchange and particle collisions. Because of the added computational expense of tracking individual particles, Eulerian-Lagrangian methods coupled with a chemistry model have only recently been applied in three dimensions (Bruchmüller et al., 2012; Li et al., 2013), but are typically limited to two-dimensional flows with a relatively small number of particles (e.g., Fletcher et al., 2000; Papadikis et al., 2009; Oevermann et al., 2009; Rabinovich et al., 2010; Wu et al., 2010). It has been demonstrated in recent work that two-dimensional simulations are only capable of capturing qualitative features of particle clustering in non-reactive flows, while a fully threedimensional description is required to accurately capture the quantitative flow behavior (Capecelatro et al., 2014a; Li et al., 2014).

In particular, it was shown in our previous work that threedimensional Eulerian–Lagrangian simulations are capable of accurately reproducing key cluster characteristics, including fall velocity, mean cluster concentration, and concentration fluctuations in risers (Capecelatro et al., 2014a).

The objective of this study is to characterize and quantify the influence of particle clusters on heterogenous reactions in systems that are applicable to a wide range of industrial systems. Fully developed three-dimensional risers are simulated via a Eulerian-Lagrangian approach, where heterogeneous reactions between the solid particles and the carrier gas phase take the form of source terms that are functions of the local solid concentration. The particles are represented as rigid spheres of diameter  $d_p$  that are significantly denser than the surrounding fluid, and heat transfer at the particle surface is neglected. In Section 2, we present a volume-filtered formalism for describing heterogenous reactions between individually tracked solid particles and the carrier gas phase. Statistics from the fully developed, three-dimensional risers are presented in Section 3. In Section 4, results from the threedimensional simulations are compared to a zero-dimensional model that solves for the temporal evolution of the average chemical species mass fraction and neglects all spatial variations. Due to non-linearities in the scalar transport equation, the zerothorder model contains a term involving the covariance between species mass fraction and particle volume fraction fluctuations. This term accounts for the effects on the chemical processes of the inhomogeneities (i.e., clusters) present in the flow and needs to be modeled. A transport equation for the fluctuating chemical source term is derived and the various contributions are presented and discussed. Finally, a presumed-shape PDF model is proposed for closure of the fluctuating chemical source term and its validity is evaluated.

#### 2. Volume filtered formalism for chemically reacting flows

#### 2.1. Transport of reactive scalars

The transport of mass fraction  $0 < \hat{Y} \leq 1$  of a chemical reactant can be fully described by

$$\frac{\partial \hat{\rho}_f \hat{Y}}{\partial t} + \nabla \cdot \left( \hat{\rho}_f \hat{Y} \, \hat{\boldsymbol{u}}_f \right) = \nabla \cdot \left( \hat{\rho}_f \hat{\mathcal{D}} \nabla \hat{Y} \right),\tag{1}$$

where the notation  $(\hat{\cdot})$  denotes a pointwise (i.e., microscale) property of the fluid phase, *t* is time,  $\hat{\rho}_f$  is the fluid density,  $\hat{u}_f$  is the fluid velocity, and  $\hat{D}$  is the diffusion coefficient. Note that because only heterogeneous reactions are considered, Eq. (1) does not contain a source term for gas-phase reactions. Instead, adsorption and desorption that occur during the chemical reaction are represented as flux boundary conditions at the particle surface. In order to formulate a tractable system of equations that does not require resolving the flow at the particle scale, a separation of length scales must be established. To achieve this, a volume filtering kernel *G* is introduced, such that the local mean value *A* of any microscale quantity  $\hat{A}$  is given by

$$\varepsilon_f A(\boldsymbol{x}, t) = \int_{V_f} \hat{A}(\boldsymbol{y}, t) G(|\boldsymbol{x} - \boldsymbol{y}) \, d\boldsymbol{y}, \tag{2}$$

where  $\varepsilon_f$  is the fluid-phase volume fraction, **y** is the location of the pointwise quantity  $\hat{A}$ , and **x** is the local coordinate system of the volume-filtered variables. Applying the volume filter to Eq. (1) yields

$$\frac{\partial}{\partial t} \Big( \varepsilon_f \rho_f Y \Big) + \nabla \cdot \Big( \varepsilon_f \rho_f \mathbf{u}_f Y \Big) = \varepsilon_f \nabla \cdot \Big( \rho_f \mathcal{D} \nabla Y \Big) - \nabla \cdot \mathbf{R}_Y + \dot{\omega}, \tag{3}$$

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