MULTISCALE MODELING OF BIOMASS PYROLYSIS IN A MULTIPHASE REACTOR: THE EFFECT OF PARTICLE SCALE MODELS ON THE SECONDARY GAS-PHASE REACTIONS.

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Abstract

Biomass pyrolysis is a complex process that requires a multiscale modeling approach to accurately model the multiphase flow reactors such as Fluidized Bed Reactors. The particle-scale models play a critical role during the pyrolysis of thermally-thick biomass particles. This work implements a multiscale modeling strategy, coupling a 1D intraparticle devolatilization model, reduced secondary gas phase reaction mechanism, and CFD-DEM simulations. The significance of particle-scale models on the secondary gas-phase reactions is assessed. To this end, we perform Drop Tube Reactor simulations in the temperature range of 973K-1273K using lumped and intraparticle devolatilization models. The secondary gas-phase reactions under these conditions are represented using a reduced chemical mechanism involving 39 species and 118 reactions. The biomass particle size and physical properties are varied to gain insights over a wide spectrum of thermal regimes. The evolution of the primary and secondary gas-phase species along the reactor is compared between the particle models. Thermal and chemical time scales are calculated to understand the competition between the particle conversion and the secondary reactions. The analysis is then extended to study the variations in a Fluidized Bed Reactor, where multiphase hydrodynamics and chemistry are coupled.

Keywords

Biomass Pyrolysis, Drop Tube Reactor, Fluidized Bed Reactor, gas-phase chemistry

Introduction

Biomass Pyrolysis involves complex processes happening at different scales within a reactor. Fluidized Bed Reactors (FBRs) are preferred for this application as they provide high heat and mass transfer rates (Bruchmu, 2011). Although the experiments provide global outputs, they fail to provide a detailed insight into the conversion process within the reactor due to the opaque nature of biomass, harsh conditions, and the deposition of tar on the measuring instruments. On the other hand, high-fidelity CFD simulations provide local and detailed information such as the particle and gas velocities and species compositions. Such a level of detail is essential to comprehend reactor behavior and predict the reactor performance.

The biomass conversion process is multiscale due to the coupling among the chemical reactions, heat, and mass transport processes at a particle level, and hydrodynamics at a reactor level (Lu et al., 2021). Particle-scale processes can impact the overall reactor performance. The homogeneous particle model, neglecting the intraparticle variations, is implemented in reactor-scale simulations due to its simplicity (Haberle et al., 2017). A few studies have recently implemented the intraparticle heat transfer effects in particle-scale models (Lu et al., 2021). In this work, we couple the homogeneous model and an experimentally validated 1D intraparticle model employing the kinetic schemes of Corbetta et al., 2014 with the CFD-DEM code NGA (Desjardins et al., 2008). The multiscale simulation framework is used to quantify the impact of particle models on the rector performance.

Methodology

The biomass conversion in a drop tube reactor (DTR) (Chen et al., 2013) is modeled using the CFD-DEM approach. Each biomass particle is tracked using Newton's second law of motion and the gas-phase equations are solved on a Eulerian grid. The homogeneous and 1D intraparticle models are integrated into the CFD-DEM code NGA to compare the particle-scale effects. A lumped devolatilization kinetic scheme with 12 solid species and 7 trapped species is included in the model to represent the solid-phase chemistry. A reduced kinetic model with 39 species and 118 reactions is implemented to represent the gas-phase chemistry (Goyal & Pepiot, 2017). The 1D intraparticle model employed in this study has been validated against experiments (Goyal & Pepiot, 2018). The biomass Biot number is set to one. The effect of particle-scale models on the yields of secondary gas phase products is studied in the temperature range of 973K to 1273K.

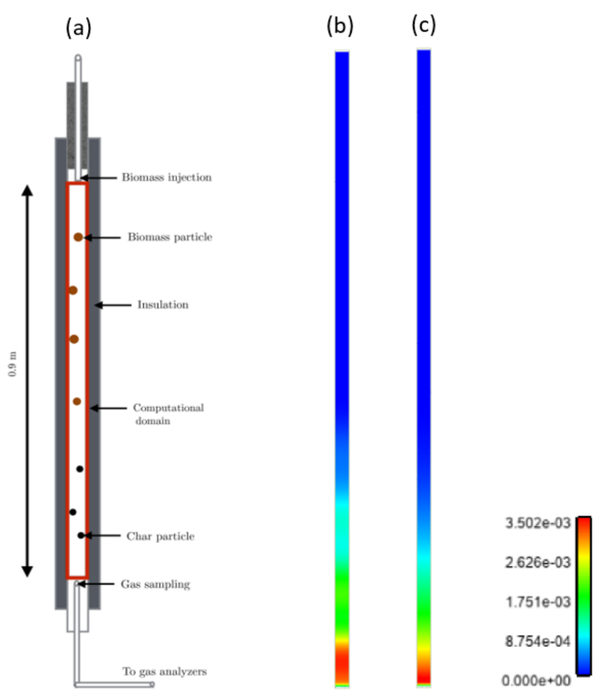

Figure 1. (a) Schematic of the drop tube experimental setup (Chen et al., 2013) implemented in this study (b) Mass fraction contour of Levoglucosan at 2 seconds using the homogeneous model at 973K (c) Mass fraction of LVG at 2 seconds using the intraparticle model at 973K.

Results

Figure 1 schematizes the DTR setup used in this study. The biomass particles and nitrogen are injected from the top of the reactor. Variations in the particle heating rate in both the particle-scale models led to differences in the composition of gaseous species along the length of the reactor. During the initial stage, the zone length containing a higher composition of LVG is greater in the homogeneous model compared to the intraparticle model as shown in Figures 1b and 1c, respectively. Biomass particles started devolatilizing at a shorter length from the inlet of the reactor in the homogeneous model compared to the intraparticle model. For this reason, the residence time for secondary gas-phase reactions varies in both cases, leading to a different product profile. (Chen et al., 2013)

Conclusion

Implementing homogeneous and intraparticle devolatilization models showed variations in production rates of primary pyrolysis products along the drop tube reactor. Slower heating rates in the intraparticle model resulted in a gradual release of primary products. In contrast, the homogeneous model predicted significantly higher heating rates, leading to the rapid release of primary products near the inlet. These variations in the species production rate impacted the secondary gas-phase reaction rates and the yields of the primary and secondary gaseous products.

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