Computational analysis of biomass particles in a bubbling bed

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Abstract

A leading candidate process for converting biomass to liquid fuels involves fast pyrolysis of the biomass in a fluidized bubbling bed reactor of inert or catalytic particles. As the biomass heats through its contact with hot gases and solids, a complex series of thermally driven reactions releases volatile constituents, ash, and char. The pyrolysis reaction rates and product gas composition, which determine the yield of fuel-compatible molecules, are highly dependent on the heat and mass transfer occurring both within the biomass particles themselves and also at the interface between the particles and their surrounding environment as they transit through the reactor.

In this study, we simulate the effects of biomass particle properties and fluidization state on the biomass particle mixing and residence time distribution in a pyrolysis reactor. For our simulations, we utilized MFIX, an open source, computational software package supported by DOE, which uses a continuum (two-fluid) approach for efficient modeling of the hydrodynamics (Garg et al. 2012, DOI: 10.1016/j.powtec.2011.09.019). We apply a novel discrete element method (DEM) algorithm to simulate the mixing behavior of individual biomass particles in a background of bed particles. The output of our simulations includes detailed statistics about the expected biomass particle trajectories.

For our initial validations, we compare our simulation results with measurements of simulated biomass particle mixing in an experimental cold-flow fluidized bed of Geldart B particles designed to replicate many of the features of a bubbling bed pyrolysis reactor. The laboratory measurements included detailed 3-D spatial trajectories of magnetically tagged simulated biomass particles in the laboratory bubbling bed (Halow et al., 2012, DOI: 10.1021/ie301517w). Comparisons are made between the simulations and experimental measurements for a range of fluidizing gas flows and biomass particle size and density. In addition, we report results from a broader parametric study with our modified MFIX model to identify general sensitivities and mixing trends in bubbling bed biomass pyrolysis reactors.