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Modeling effects of interphase transport coefficients on biomass pyrolysis in fluidized beds

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ABSTRACT

This study numerically characterizes the effects of interphase transport coefficients on the simulation of biomass pyrolysis in fluidized-bed reactors. Numerical modeling of sub-grid structures can affect the evolution of interphase transport coefficients and influence the predictive capability of coarse-grid computational fluid dynamics (CFD) models in simulating fluidized-bed reactors. In this study, a multi-fluid model that solves mass, momentum, energy and species conservations was coupled with chemical reactions to simulate a laboratory-scale biomass fast pyrolysis reactor. Different formulations of drag and heat transfer coefficients were employed. Comparisons between the simulated and experimental results show that the drag coefficient model considering detailed sub-grid structures predicted lower drag forces and performed better than the homogeneity-based drag correlation models. Lower drag forces on solid biomass particles resulted in lower solid biomass outflux, higher gas velocities, and shorter tar residence time, all resulting in higher tar yields. On the other hand, heat transfer correlations had less effect on the temperature distributions and final product yields. These findings indicate that when coarse-grid CFD is used to simulate biomass fast pyrolysis in fluidized-bed reactors, effects of sub-grid structures need to be taken into account in the formulations of drag coefficients.

1. Introduction

Bio-oil, derived from fast pyrolysis of biomass, has the advantages of high energy density, low transportation cost, and direct applications in combustion devices [1]. With the increasing concern regarding availability and environmental impacts of fossil fuels, bio-oil has attracted increased interest in recent years [2]. Fast pyrolysis, a thermochemical conversion process in the absence of oxygen, has served as the dominant means of converting lignocellulosic biomass to bio-oil. Developing highly efficient fast pyrolysis technologies, crucial to bio-oil production, has therefore received extensive interest [3].

Experimental study has been the main approach to developing advanced technologies for biomass fast pyrolysis [4]. However, performing experiments at different scales (e.g., laboratory scale, pilot scale, and industry scale) is usually time-consuming, making this approach cost ineffective. The accuracy of measurements in the hostile reactor environment also poses great challenges. In contrast, numerical simulation can complement experiments into the fundamental details of the reactor processes [5]. An accurate numerical model can be used to investigate the effects of operating variables on the reactor performance and can shorten the development cycle considerably. As a result, numerical simulations are increasingly conducted to study phenomena inside the biomass pyrolysis reactors [6].

Specific to the computer simulation at the reactor scale, process modeling [7–9] and computational fluid dynamics (CFD) [10–13] have been the main choices so far. Although process modeling is capable of predicting product yields and overall performance much more quickly than CFD, it does not provide detailed information on processes occurring inside reactors, such as tempo-spatial distributions of voidage, velocity, temperature, and species mass fractions. This information is critical to reactor operation and design. Because CFD discretizes the reactor into an ensemble of grids where conservation equations for mass, momentum and energy are solved, temporal evolutions at every location can be provided. On the basis of such useful details on what occurs inside the reactor, more guidelines can be developed and applied to designing industrial reactors. Furthermore, because of the continuum description of the solid phases, as is true for the gas phase, using CFD has been proven to be a good compromise between the computational requirement and model applicability. Therefore, the continuum-based CFD approach has become increasingly important in studying biomass pyrolysis in fluidized-bed reactors [14–20].

In CFD simulations of single-phase flows, the predictive capability largely depends on the grid size employed. With the rapid increase of computer power, reducing grid size for improved resolution of solutions is not difficult to attain. It has been argued that the predictive capability of continuum-based CFD simulations of multi-phase flows can be improved by merely choosing sufficiently small meshes [21]. However, some critical phenomena, e.g., the S-shape distribution of solid volume fraction in circulating fluidized beds, cannot be reproduced in gas–

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solid flows in circulating fluidized beds even with extremely small meshes [22]. A possible explanation is that the continuum assumption for simulating the solid phase in CFD requires a relatively large grid size, below which sub-grid heterogeneous structures such as particle clusters inevitably exist [23]. It was also demonstrated that sub-grid structures significantly influence the formulations and magnitudes of the interphase transport which appear in the simulations of multiphase, gas–solid flows [24,25]. This dilemma implies that although it is only reasonable to use a coarse computational grid, the effects of sub-grid structures on the interphase interactions should be taken into account. That is, revisited interphase transport coefficient models considering the effects of subgrid structures should be employed in conjunction with coarse-grid discretization of the simulation domain. In other words, choosing proper interphase transport coefficient models becomes the critical point in the coarse-grid CFD simulations of gas–solid flows. For unreactive gas–solid flows, the effects of subgrid structures on the interphase transport coefficients have received considerable attention in recent years [26]. Li and Kuipers [27] compared several drag models in the continuum-based CFD simulation of a dense gas–solid flow and pointed out that the predicted flow behaviors are highly sensitive to the formulations of drag models which are implicitly affected by the effects of subgrid structures. This finding was confirmed by Hartge et al. [28]. Therefore, great efforts have been paid to deriving appropriate interphase transport coefficient models to account for the effects of subgrid structures in coarse-grid simulations. Agrawal et al. [29] and Igci et al. [30,31] have developed a method that deriving filtered interphase transport coefficient models from fine-grid simulations. The filtered interphase transport coefficient models were found to perform much better than those without inclusion of the effects of subgrid structures [32,33]. Another approach is that using analytical methods such as the so-called EMMS theory to account for the effects of subgrid structures on interphase transport coefficients, by decomposing the subgrid structures into dense and dilute regions [34,35]. This strategy also led to a remarkable success in nonreactive gas–solid flow simulations using coarse-grid CFD [36,37]. However, the dependence of CFD modeling on the interphase transport coefficients, which are implicitly affected by the sub-grid structures, have rarely been clarified in the gas–solid flow simulations of fast pyrolysis reactors. So far, almost all the continuum-based CFD simulations of biomass pyrolysis in fluidized-bed reactors have used standard homogeneity-derived closures for interphase transport coefficients, such as Gidaspow drag [38] for gas–solid momentum transfer and Ranz–Marshall convection [39] for gas–solid heat transfer. Therefore, it is necessary to characterize the effects of the interphase transport coefficient models on modeling accuracy and develop improved CFD models for reactor design and optimization of biomass fast pyrolysis.

In this study, different correlations for the interphase transport coefficients are investigated and their effects on the performance of a fluidized-bed reactor for biomass pyrolysis are characterized. A comprehensive multi-fluid model (MFM) that describes the hydrodynamics of gas, sand, and solid biomass is coupled with chemical reactions for simulating biomass fast pyrolysis in the reactor. The results are compared with experimental data to assess the performance of various correlations.

2. Model formulation

A comprehensive multi-fluid model, a variant of the two-fluid model [40], is employed to simulate the hydrodynamics of a fluidized-bed reactor [41,42]. Different from other numerical methods for simulating fluidized beds such as direct numerical simulation [25,43,44] and discrete particle simulation [45,46] where solid phases are represented by discrete objects and the motions of the solid particles are tracked individually, MFM models gas and solid phases as interpenetrating continua and describes each phase by a set of volume fraction incorporated conservation equations. The conservation equations for mass, momentum, energy, and species in each phase are summarized in Table 1. The modified multi-component multi-stage Broido–Shafizadeh reaction kinetics is chosen for the biomass fast pyrolysis reactions [47], as shown in Fig. 1. In this reaction mechanism, biomass is assumed to be composed of cellulose, hemicellulose and lignin, and the mass fraction of each component is specified. When fast pyrolysis starts, each component is activated into an intermediate stage, followed by two competitive decomposition reactions that yield tar, char and gas. At appropriate temperature and reactor conditions, some portion of tar further decomposes into gas. The rate of each reaction is controlled by first-order Arrhenius kinetics. A parametric study has shown that this reaction kinetics is able to reproduce the biomass decomposition accurately [48]. Detailed description of the MFM and the parameters in the pyrolysis reaction kinetics can be found in [41,47]. The above conservation equations and the chemical reaction kinetics are solved using our developed open-source code, BIOTC (BIOmass Thermochemical Conversion) [41] developed based on the OpenFOAM® platform. A comparative study [49] has proved that OpenFOAM® can produce equivalent results as those by MFIX and Fluent®. In BIOTC, all the conservation equations are discretized by finite volumes and solved by the so-called PIMPLE method, a combination of the popular PISO and SIMPLE methods to obtain the tempo-spatial evolutions of phase physical variables, e.g., phase volume fraction α. The time derivative terms, gradient terms, divergence terms, and Laplacian terms are discretized by the first-order accuracy bounded Euler scheme, second-order accuracy Gauss scheme, second-order accuracy bounded TVD scheme, and second-order accuracy corrected scheme. The effects of turbulence were modeled by the standard $k-\varepsilon$ two-equation model [50].

The hydrodynamic coupling between the gas and solid phases is realized by the interphase transport coefficients appearing in both the momentum and energy conservation equations. As the drag force plays a dominant role in the gas–solid momentum transfer, only drag correlations are considered in the phase momentum equations. For the gas–solid heat transfer, only convective heat transfer is accounted for. Three typical correlations for the gas–solid drag force and three typical correlations for gas–solid heat transfer are considered in this study. The formulations of these interphase transport coefficients are listed in Tables 2 and 3. For convenience, these interphase models are referred to as D1 for the Gisaspow model [38], D2 for the Syamlal-O'Brien model [51], D3 for the EMMS model [22], H1 for the Ranz-Marshall model [39], H2 for the Gunn model [52], and H3 for the Li-Mason model [53].

3. Simulation conditions

A lab-scale bubbling fluidized-bed reactor located in the Agricultural Research Service (ARS) of the U.S. Department of Agriculture (USDA) was simulated [54]. The configuration of the reactor is shown in Fig. 2, which includes geometry and boundary conditions. The fluidization medium was silica sand, initially packed to a height of 17 cm and porosity of 0.45. The biomass feedstock, switchgrass, was fed from the side injector at the left, located 5 cm from the bottom, at a feed rate of 2.22 kg/h. The initial composition of switchgrass is assumed to be 42% cellulose, 34% hemicellulose, and 24% lignin [16]. Fluidization nitrogen was supplied from the bottom of the reactor at a fixed rate of 4.81 kg/h. The sidewall was heated and maintained at a fixed temperature of 773 K. The physical properties of each species in each phase are listed in Table 4.

To reduce computational effort, a two-dimensional (2-D) domain was simulated. As demonstrated in our previous study [42] and that by Xue et al. [18], 2-D simulation can provide results comparable to those of its 3-D counterpart. The domain was meshed into 30×200 grids in the radial and axial directions, respectively. Preliminary studies have shown that this mesh size was appropriate to give