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Multi-fluid model with variable particle density and diameter based on mass conservation at the particle scale

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ABSTRACT

The multi-fluid model (MFM) has been widely used in the simulation of gas–solid fluidized bed reactor, in which the density and diameter of particles normally change due to the heterogeneous reactions. However, the particle diameter always keeps constant although the particle density varies along with reaction in the previous MFM, which may disobey the law of mass conservation at the particle scale. Therefore, in order to overcome the limitation of constant diameter in the previous MFM, the biomass pyrolysis reaction was taken as an example to develop the variable particle density and diameter model based on the mass conservation at the particle scale, which was successfully incorporated into MFM to simulate the biomass pyrolysis process in a fluidized bed reactor. The results indicate that the segregation/mixing and entrainment behavior are significantly affected by the variation model of particle density and diameter and the species density in the solid phase.

1. Introduction

Gas–solid fluidized bed reactors are widely used in the chemical industry due to their excellent heat and mass transfer characteristics. In the gas–solid fluidized bed reactors with heterogeneous reactions such as pyrolysis, combustion, and gasification of solid fuel particles (coal, biomass, etc.), the density and diameter of particles normally change with the process of reaction. It is well-known that the hydrodynamics of gas–solid fluidized bed such as segregation/mixing and entrainment behavior are severely affected by the particle density and diameter. Therefore, the variation of particle density and diameter due to the heterogeneous reaction should be carefully considered when investigating the characteristics of hydrodynamics and reaction in the gas-fluidized bed reactor.

Recently, computational fluid dynamics (CFD) has been increasingly employed as an efficient tool to investigate the complex hydrodynamic and reaction behavior of gas–solid fluidized bed reactor with the rapid development of CFD model and computational ability. Typically, there are two different CFD methods for the simulation of gas–solid fluidized bed reactor, i.e., the Eulerian–Lagrangian method and Eulerian–Eulerian method. For both methods, the gas phase is described using the continuum equations, while the solids are handled by different methods. In the Eulerian–Lagrangian approach, the particle phases are described by tracking the motion of individual particles, and the detailed forces exerted on each particles can be simulated, while the solids are considered as fully interpenetrating continua subject to continuity and momentum equations in the Eulerian–Eulerian method. The Eulerian–Eulerian method, which also named as two-fluid model (TFM) or multi-fluid model (MFM) for more than one solid phase, has been widely used in the CFD simulation of gas–solid fluidized bed reactor, such as biomass pyrolysis [1–3], coal combustion [4–6] and gasification [7–10], fluid catalytic cracking (FCC) riser [11–13], and polymerization reactors [14,15]. In order to improve the TFM or MFM, many efforts have been made in recent years, such as the subgrid drag modifications for mesoscale structures [16–20] and the description of particle–wall interaction [21–25]. However, when applying TFM or MFM to simulate the gas–solid fluidized bed reactor with variable particle density and diameter due to the heterogeneous reactions, less attention have been paid to the variation of particle density and diameter in the CFD model.

In the CFD modeling of gas–solid fluidized bed reactor with TFM or MFM, there are two different methods to account the solid species. One method treats the solid reactant (e.g. coal) and product (e.g. char) as different solid phases with fixed density and diameter [8,9], which is hard to reflect the continuous variation of particle density and diameter in the real reactor. The other method defines the reactive solid phase containing all the solid species in the heterogeneous reaction, and the density of solid phase is defined by the mixing law according to the composition of solid species [1,3,4]. For example, when modeling the pyrolysis reaction of biomass, the bio-mixture phase contains two

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solid species, i.e., biomass and char, and the density of bio-mixture is calculated using Eq. (1) [1,3].

$$\rho_{sm} = \frac{1}{\frac{Y_b}{\rho_b} + \frac{Y_c}{\rho_c}} \tag{1}$$

where ρ_{sm} is the density of bio-mixture phase. Y_b and Y_c are the mass fraction of biomass and char, respectively. ρ_b and ρ_c are the density of pure biomass and char species, respectively.

Hence, the density of bio-mixture varies during the biomass pyrolysis reaction. However, the diameter of bio-mixture always keeps constant with the explanation of the constant particle size during chemical reaction [3] or the restriction of Eulerian–Eulerian model [9], and there is no relation between the particle density and diameter at the particle scale since the mass conservation of particles during heterogeneous reactions are only applied on the grid cell instead of individual particles due to the interpenetrating continua assumption of solids in the Eulerian–Eulerian method. This is different with the Eulerian–Lagrangian approach in which the particle diameter and density can be related through the mass conservation on the tracked individual particles. Unfortunately, the variable particle density and constant diameter treatment for the reactive solid phase in the TFM or MFM may disobey the law of mass conservation at the particle scale during the heterogeneous reaction. For example, assuming the fresh biomass particle with density of 400 kg/m^3, and after complete pyrolysis reaction all biomass were transformed to char with density of 2330 kg/m^3, according to Eq. (1) the bio-mixture density changes from 400 kg/m^3 to 2330 kg/m^3. If the particle diameter keeps constant, for a single fresh biomass particle, its mass will increase after the pyrolysis reaction although some gas products were released, which apparently disobey the law of mass conservation at the particle scale as shown in Fig. 1a. Although this violation of mass conservation at the particle scale does not affect the mass conservation in the computation domain (grid cell) due to the continua treatment of solid phase in the Eulerian–Eulerian model, the equations containing particle density and diameter such as gas/solid–solid interaction and solid phase properties may be wrongly calculated, which may affect the predicted hydrodynamic and reaction behavior. Therefore, in order to correctly determine the particle density and diameter during the heterogeneous reaction, the variable density and diameter model should be developed based on the mass conservation at the particle scale as shown in Fig. 1b. However, as far as we know, no reference for CFD simulation of gas–solid fluidized bed reactor using TFM or MFM with variable diameter model has been reported.

In the present work, the biomass pyrolysis process in a fluidized bed reactor was taken as an example to illustrate the procedure for developing the variable density and diameter model based on the law of mass conservation at the particle scale. The variable density and diameter model was successfully incorporated into the MFM to describe the variation of particle density and diameter during the pyrolysis reaction, which overcomes the limitation of constant diameter in the previous MFM with variable density and constant diameter. The segregation/mixing and entrainment behavior were used to reveal the differences between the developed variable density and diameter model and the previous variable density and constant diameter model, and the effect of char density in the variable density and diameter model was also investigated.

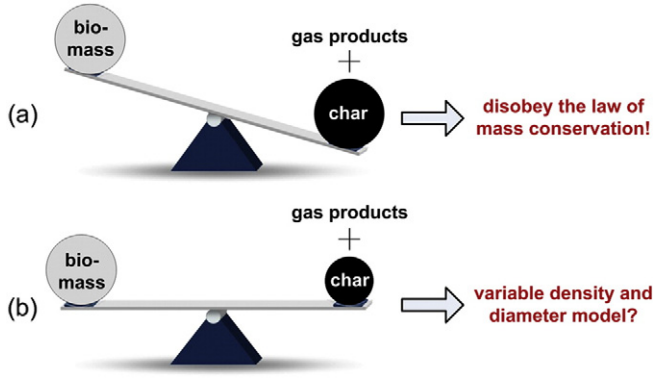

Fig. 1. Mass conservation at the particle scale.

2. Model description

The mechanism of biomass pyrolysis reaction was described by the kinetic model. The variable particle density and diameter model was derived based on the law of mass conservation at the particle scale. Both kinetic model and variable density and diameter model were successfully incorporated into the MFM for CFD simulation of biomass pyrolysis process in a fluidized bed reactor.

2.1. Kinetic model

Although the complex biomass pyrolysis mechanism including three competition reaction routes for the pyrolysis reaction and tar secondary reaction has been used in the previous reports [2,3] it is hard to describe this complex biomass pyrolysis mechanism using chemical equations with certain chemical formulas and stoichiometric coefficient. Therefore, a simplified reaction mechanism of biomass pyrolysis was used in the present work analogous to the coal pyrolysis reaction [4,9]. Char, tar, and light gas were obtained after biomass pyrolysis through one-step reaction as shown in R1.

$$\text{biomass} \rightarrow x_c\ \text{char} + x_t\ \text{tar} + x_g\ \text{light gas} \tag{R1}$$

where x is the mass fraction of pyrolysis products with $x_c = 27.0$ wt.%, $x_t = 28.0$ wt.%, and $x_g = 45.0$ wt.% [26]. Assuming char and tar contain pure C and C_8H_{18}, respectively, the pyrolysis equation with certain chemical formulas and stoichiometric coefficients was obtained from R1 and the composition of light gas [26,27]:

$$C_{52.04}H_{77.75}O_{18.63} \rightarrow 22.5C + 2.46C_8H_{18} + 4.338CO + 3.947CO_2 + 1.575CH_4 + 7.2H_2 + 6.399H_2O. \tag{R2}$$

The biomass pyrolysis reaction was modeled with the first-order Arrhenius kinetics depending on the rate constant (A), activation energy (E), and temperature (T):

$$k = Ae^{-E/RT} \tag{2}$$

where $A = 1.30 \times 10^8$ 1/s, $E = 1.403 \times 10^8$ J/kmol [26].

2.2. Variation model for particle density and diameter

For simplicity, the variable density and constant diameter model in previous MFM is named as “default model”, and the variable particle density and diameter model in the present work derived by the mass conservation at the particle scale is named as “both-vary model”. In addition, the special cases for constant density and constant diameter in the both-vary model are named as “size-vary model” and “density-vary model”, respectively. The present work focused on the variation of particle density and diameter caused by the heterogeneous reaction, and the particle breakage and attrition were neglected.

2.2.1. Default model

In the default model, the density of bio-mixture phase is calculated using Eq. (1), while the diameter of bio-mixture keeps constant during the simulation.