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A Multi-scale Model for the Simulation of Bubbling Fluidized Bed Methanation

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Highlights

- A multi-scale model is developed to describe the fluidized bed mathanation process.
- The multi-scale model includes the micro-scale, meso-scale and macro-scale models.
- This model can accurately predict the bed expansion height of a lab-scale reactor.
- The simulated concentration of each species is in agreement with the experimental data.

1. Introduction

Methanation of synthesis gas or lignocellulosic biomass to produce synthetic nature gas (SNG) is suitable to occur in a bubbling fluidized bed due to its excellent heat and mass transfer performances [1]. However, the inherent complexity of gas-solid two-phase flow and the highly exothermic chemical reactions in the fluidized-bed methanation process would make it difficult to design and scale up of the reactors [2]. At present, the computational fluid dynamics (CFD) is a powerful tool to reveal the hydromechanics behaviors and the chemical reactions in the reactors.

However, the multi-scale phenomenon in the bubbling fluidized bed makes it complex to simulate the methanation process. The micro-scale includes the CO mehanation reaction and water gas shift reaction taking place in a single catalyst particle. The chemical reactions can not only change the concentration of each species but also generate considerable energy source and contract the volume gas phase. The meso-scale contains the gas-rich bubble phase and particle-rich emulsion phase. The existence of such heterogeneous flow structure leads to the gas-solid drag reduction compared with the conventional uniform drag force [3]. The macro-scale includes the momentum, heat and mass transfers in the bulk gas and bulk solid if the two-fluid model (TFM) is employed to simulate the whole process. In this work, a multi-scale model is established to simulate the fluidized bed methanation process and this model is verified by a lab-scale fluidized bed reactor.

2. Methods

In the micro-scale, CO methanation reaction and water gas shift reaction are considered. The reaction kinetics of Kopyscinski et al. [4] is adopted to calculate the rates of both reactions.

In the meso-scale, the heterogeneous flow structure is taken into account to describe the gas-solid interaction in the bubbling fluidized bed. The extended bubble-based energy-minimization multi-scale (EMMS) model in our previous work [5] is used to account for the influences of the meso-scale structure and chemical reactions on gas-solid interaction. Here, the gas physical properties (density and viscosity) changes spatially in a reactor because of the variations of composition and temperature of gas phase caused by the chemical reactions. Therefore, the impacts of gas properties on the drag force should be evaluated.

In the macro-scale, the TFM is applied to simulate the gas-solid flow structure. Meanwhile, the energy conservation equation and species transport equations are used to reveal the heat and mass transfers, respectively.

Furthermore, the coupling of the three scales is carried out to close the conservation equations in the macro-scale. The meso-scale model is the closure law of the momentum equations in the TFM model; the reaction kinetics and heat-effect in the micro-scale are used to close the species transport equations and the energy conservation equation, respectively.

Then, the multi-scale model is verified by a lab-scale bubbling fluidized bed [1].

3. Results and discussion

It can be observed from Figure 1 that the influence of gas viscosity is dominated. Thus, the heterogeneity index of the drag force is expressed as a function of the gas voidage and viscosity.

The grid independence of the multi-scale model is studied and the results are shown in Figure 2. It can be observed that the solutions are nearly unchanged with the increase of grid resolution. Meanwhile, the simulated bed expansion height is consistent with the experimental data. This indicates that the multi-scale model can provide satisfying accuracy for the hydromechanics behaviors in a fluidized bed.

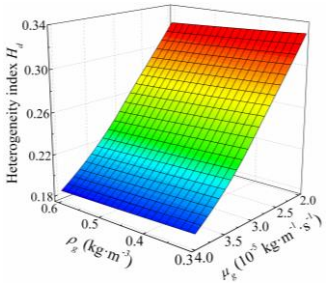

Figure 1. The influence of gas properties on drag force.

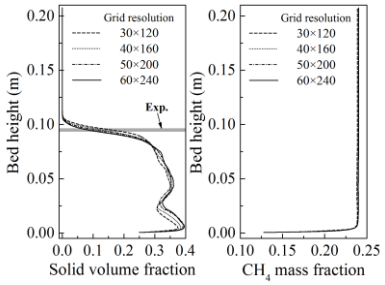

Figure 2. Grid independence and comparison with experimental data.

The verification of the simulation results for the chemical reactions behavior is shown in Figure 3. In general, the simulated concentration of each species is in agreement with the experimental data at higher bed height. However, the obvious discrepancy between the simulation results and the experiment data is observed near the inlet of the reactor. This is probably because the methanation reactions mainly take place near the distributor and this will lead to an obvious temperature increase. In contrast, the temperature increase was not predicted in our simulations. Therefore, the reaction rates of the experiment are higher than those of the simulation near the inlet.

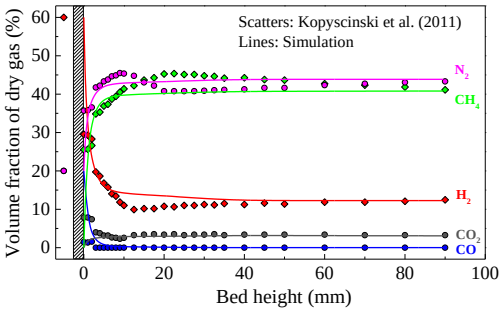

Figure 3. Comparison of the simulated and experimental concentration of each species.

4. Conclusions

In this work, a multi-scale model is developed to describe the hydromechanics behaviors and the chemical reactions in the bubbling fluidized bed methanation process. The experimental data from a lab-scale reactor is used to verify the multi-scale model. The simulation results indicate that the multi-scale model is capable to predict the bed expansion height and the axial concentration distribution of each species.

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Keywords
Bubbling fluidized bed; Methanation reactions; Multi-scale model; CFD Simulation