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CFD analysis of bubble column reactor under gas–oil–water–solid four-phase flows using Lagrangian algebraic slip mixture model

Zhi Shang*, Jing Lou, Hongying Li

*Institute of High Performance Computing, Agency for Science, Technology and Research (A*STAR), 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632, Singapore*

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ABSTRACT

A Lagrangian algebraic slip mixture model (LASMM) has been developed to study gas–oil–water–solid four-phase flow. In this model the slip velocities between continuous and dispersed phases were derived from the Lagrangian movement equation. Therefore the slip velocities are able to consider the effects of various interfacial forces, such as buoyancy, drag, lift, virtual mass and turbulent dispersion. This model is easily coded through the user defined functions (UDFs) linking to the commercial or open source software. The validations were carried out through the comparisons of the numerical simulations to the experiments of gas–water–solid and gas–oil–water three-phase flows. For the validations of gas–water–solid three-phase flows, the simulation results compared to Michele and Hempel's (2002) experiments on a cylindrical bubble column reactor. The comparisons were carried out by the quantitative comparisons on the axial water velocity under different inlet superficial gas velocities. For the validations of gas–oil–water three-phase flows, the simulation results compared to Descamps et al.'s (2007) experiments on a vertical pipe. The comparisons were performed by the quantitative comparisons of the gas volume fractions at different water cuts under different inlet flow conditions. After the validations, this model was used to study the gas–oil–water–solid four-phase flows in the bubble column reactor. The distributions of the solid phase and gas phase under different situations of oil-in-water and water-in-oil flows were studied. It was found that following the increase of the water cuts, in the oil-in-water flows, the solid particles were pushed away from the center of the column; however the solid particles were absorbed into the center of the column in the water-in-oil flows. The CFD work evaluates the aptness of the LASMM to predict the motion of a gas–oil–water–solid mixture to further the understanding of such complex reaction processes.

Introduction

In engineering, multiphase flow can be encountered in many industrial processes such as fluidized beds, coal combustion boilers, food and commodity transfers, solid rocket jets, pharmaceutical granulators, the dryers and filters in oil & gas industry. In multiphase flow system, the dispersed phases are usually transported by the continuous phase. In the dispersed phases, the gas phase normally is formed as bubbles, the liquid phase is formed as droplets and the solid phase is grounded into fine powder. During the flow processing, bubbles and droplets have not only the deformable shapes but also have coalescence and breakup. The solid powders not only have the interactions with continuous phase but also have collisions with each other. Therefore the flow phenomena of multiphase flows are very complex.

Understanding the complexity of the fluid dynamics in bubble column and airlift reactors is important because of their application in the chemical and bioprocess industries. Knowledge of the hydrodynamics of such reactors helps to determine the efficiency of chemical production rates through transport processes such as inter-phase gas transfer, mixing of catalysts and reactants. Many parameters control the flow of solid and fluid phases through bubble column and airlift reactors, where the relative buoyancy of each discrete phase is the major driving force applied to the flow regime. Other factors such as surface tension, viscosity and density can affect the complex flow phenomena include the coalescence and disruption of droplets and bubbles. The values of those parameters can also influence the volume fraction of the bubbly gas phase and granular solid phase. Therefore, to improve the efficiency of multiphase reactors, the dynamic interactions between the discrete and continuous phases must be understood (Glover and Generalis, 2004).

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* Corresponding author.
E-mail addresses: shangzhi@tsinghua.org.cn, shangz@ihpc.a-star.edu.sg (Z. Shang).

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The experimental methods usually were employed to explore the complex internal flow structure of multiphase flows. Ruck and Makiola (1988) used laser-Doppler anemometry (LDA) to measure the velocity distributions of solid particles behind the backward-facing step in gas–solid two-phase flows, shown in Fig. 1. Michele and Hempel (2002) employed the invasive measurement technique called electrodiffusion measurement (EDM) to measure the liquid velocity in gas–water–solid three-phase flows. Sun et al. (2004) used laser-Doppler anemometry (LDA) to study the upward and downward air–water two-phase flows and found the phase distributions in the upward and downward flows were indeed quite different. Descamps et al. (2007) employed the optical fiber probes and high speed video recording technology to measure and track the bubbles in gas–oil–water three-phase flows. From experiments, the flow structure and specific physical parameters can be measured directly. However, the cost of doing experiments is very high. Using the advantage of computer technology, the flow structure and specific physical parameters of multiphase flows can be simulated numerically based on computational fluid dynamics (CFD) methodology (Shang, 2005; Pakhomov et al., 2007; Verma et al., 2013).

However the accuracy of CFD will depend on the models. Currently the mixture, two-fluid and Eulerian–Lagrangian models are able to perform the numerical simulations for multiphase flows (Shang, 2005; Zhang et al., 2006; Hernandez-Jimenez et al., 2011). Within these models, Eulerian–Lagrangian model is accurate but the computing cost is high; the two-fluid model is popular but complex; the mixture model is simple but the accuracy is difficult to be guaranteed. In the mixture model, the algebraic slip mixture model (ASMM) is often employed to simulate multiphase flows. In traditional ASMM, the interfacial forces such as drag force, lift force, virtual mass force and turbulent dispersion force are not included. Hence the accuracy of the traditional ASMM will be affected (Shang et al., 2013, 2014).

A Lagrangian algebraic slip mixture model (LASMM) was developed in this paper for multiphase flow according to the former studies by the authors for two-phase flows (Shang et al., 2013, 2014). It employed a mixture model to describe the multiphase flows based on the Eulerian model. The slip velocity, which can be developed from the dynamic equation of the dispersed phase based on Lagrangian model, was introduced to represent the velocity difference between dispersed and continuous phases. Owing to the Lagrangian model, the interfacial forces, such as buoyancy, drag, lift, virtual mass and turbulent dispersion, are able to be involved. Therefore the LASMM overcomes the disadvantages of low accuracy of the traditional mixture model. Through the comparisons to experiments and two-fluid model on gas–solid–water and gas–oil–water three-phase flows, this model was validated. Based on the validations, the gas–oil–water–solid four-phase flows in the column reactor were studies numerically. Through the investigations, it was found that the different liquid dispersed phase will have evident effects on the distributions of the gas phase and solid phase in the gas–oil–water–solid four-phase flow systems.

Mathematical model

The time averaged conservation equations of mass, momentum and energy as well as the turbulent kinetic energy equation and the turbulent kinetic energy transport equation for the mixture model can be described as follows. The flow system is of a turbulent multi-component multi-phase flow with one continuous phase and several dispersed phases.

$$\partial\rho_m/\partial t + \nabla\cdot(\rho_m\mathbf{U}_m) = 0 \tag{1}$$

$$\begin{aligned}\partial(\rho_m\mathbf{U}_m)/\partial t + \nabla\cdot(\rho_m\mathbf{U}_m\mathbf{U}_m) = {} & -\nabla p + \rho_m\mathbf{g} \\ & + \nabla\cdot\left[(\mu_m+\mu_t)\left(\nabla\mathbf{U}_m + \nabla\mathbf{U}_m^T\right)\right] \\ & - \nabla\cdot\sum\alpha_k\rho_k\mathbf{U}_{km}\mathbf{U}_{km}\end{aligned} \tag{2}$$

$$\partial(\rho_m k)/\partial t + \nabla\cdot(\rho_m\mathbf{U}_m k) = \nabla\cdot\left[\left(\mu_m + \frac{\mu_t}{\sigma_k}\right)\nabla k\right] + G - \rho_m\varepsilon \tag{3}$$

$$\begin{aligned}\partial(\rho_m\varepsilon)/\partial t + \nabla\cdot(\rho_m\mathbf{U}_m\varepsilon) = {} & \nabla\cdot\left[\left(\mu_m + \frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\right] \\ & + \frac{\varepsilon}{k}(C_1G - C_2\rho_m\varepsilon)\end{aligned} \tag{4}$$

in which

$$\rho_m = \sum\alpha_i\rho_i \tag{5}$$

$$\mu_m = \sum\alpha_i\mu_i \tag{6}$$

$$\rho_m\mathbf{U}_m = \sum\alpha_i\rho_i\mathbf{U}_i \tag{7}$$

$$\mathbf{U}_{im} = \mathbf{U}_i - \mathbf{U}_m \tag{8}$$

$$G = \frac{1}{2}\mu_t\left(\nabla\mathbf{U}_m + \nabla\mathbf{U}_m^T\right) : \nabla\mathbf{U}_m \tag{9}$$

$$\mu_t = C_\mu\rho_m\frac{k^2}{\varepsilon} \tag{10}$$

where subscript m is mixture, i is the ith phase, ρ is the density, $\mathbf{U}$ are the velocity vectors, α is the volumetric fraction, p is pressure, $\mathbf{g}$ is the gravitational acceleration vector, $\mathbf{U}_{im}$ is the diffusion velocity vector of the ith phase relative to the averaged mixture flow, μ is viscosity, μ_t is turbulent viscosity, G is stress production. C_μ, σ_k, σ_ε, C_1, C_2 are constants for standard $k-\varepsilon$ turbulence model (Launder and Spalding, 1974), shown in Table 1.

Additional to the above equations, the following conservation equation for each phase is also necessary.

$$\partial(\alpha_i\rho_i)/\partial t + \nabla\cdot(\alpha_i\rho_i\mathbf{U}_m) = \Gamma_i - \nabla\cdot(\alpha_i\rho_i\mathbf{U}_{im}) \tag{11}$$

where Γ_i is the generation rate of the ith phase.

In order to obtain closure of the governing Eqs. (1)–(11), it is necessary to determine the diffusion velocities $\mathbf{U}_{im}$. The following

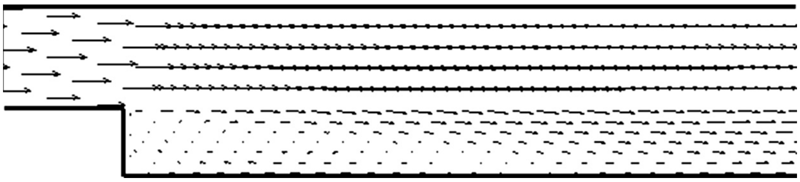

Fig. 1. Backward facing step diagrammatic sketch.