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A multi-dimensional Lagrangian algebraic slip mixture model for bubble column reactors

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ABSTRACT

A multi-dimensional Lagrangian algebraic slip mixture model has been developed to study multiphase flows. Through the single bubble Lagrangian movement equation, this model considers the accelerations of various forces on the bubble. Accordingly the slip velocities between bubbles and liquid were derived in Lagrangian manner to connect the effects of the various forces on bubbles with the diffusion flux velocities which appear in the Euler governing equations. Therefore this model realizes the connection between Eulerian model and Lagrangian model. Because the single bubble Lagrangian movement was extended to multi-dimension, the model is able to describe multi-dimensional movement of multiphase flows. Through the numerical simulations comparing with the experiments and the simulations of other models on bubble columns, the model is validated.

1. Introduction

Bubble column reactors are widely used as gas–liquid and gas–liquid–solid contactors in many chemical, petrochemical and biochemical industries, such as absorption, oxidation, hydrogenation, catalytic slurry reaction, coal liquefaction, aerobic fermentation. The operation of these reactors is preferred because of the simple construction, ease of maintenance and low operating costs. When the gas is injected at the bottom of the column, it causes a turbulent stream to enable an optimum gas exchange. It is built in numerous forms of construction. The mixing is done by the gas sparging and it requires less energy than mechanical stirring. The liquid can be in parallel flow or counter-current. Usually the bubble column is particularly useful in reactions where the gas–liquid reaction is slow in relation to the absorption rate.

A good understanding of the liquid dynamics of a bubble column will help the engineers to design a high efficient reactor under optimized operating parameters. Due to the complex two-phase or multi-phase flow and turbulence, normally the flow in bubble columns is under transient regime. The time average values of the parameters, such as gas holdup distributions, liquid phase back mixing, gas–liquid interface disturbing, mass and heat transfer between gas and liquid phases, bubble size distributions, bubble rise velocities etc., have to be considering the influence of turbulence. Although the operation of bubble columns is simple, the actual physical flow phenomena are still lack of complete understanding of the fluid dynamics [1].

Many experimental facilities and methods were introduced to study the multiphase flows in bubble columns. Krishna and Baten [2] used a modified Pitot tube, called as Pavlov tube, method to measure the liquid velocities and radial profiles. Sanyal et al. [1] used computer automated radioactive particle tracking (CARPT) method to directly measure the time-average

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velocity and turbulence parameters of the liquid phase in the bubble column. Zhou et al. [3] used charge-coupled device (CCD) camera equipped with a variable electronic shutter to record the image of the flow field. The experimental methods can provide very useful information about the bubble columns at certain measurement points, but they are difficult to show the details of the flow fields and parameters inside the bubble columns.

Following the development of computer technology, it is already allowed to use the numerical method to do the researches in the recent decades [4]. Therefore, many researchers employ the numerical method, called as computational fluid dynamics (CFD), to study the details of the flows inside bubble columns. Sanyal et al. [1] employed the algebraic slip mixture model (ASMM) and Euler–Euler two-fluid model provided by FLUENT commercial software to simulate a cylindrical bubble column from bubbly flow regime to churn flow regime respectively and compared with experiments. Zhou et al. [3] developed a second-order moment turbulence model based on Euler–Euler two-fluid model. Through comparisons with experiments, this model shows a good agreement on turbulent kinetic energy of fluid flows. However it has to deal with complex turbulence modeling. Zhang et al. [5] employed Euler–Euler two-fluid model provided by CFX commercial software to simulate a rectangle bubble column. They found the interfacial force coefficients had evident influences on the simulations. Through the former studies of CFD method, it can be seen a good mathematical model will not only help to obtain the agreeable simulation results, but also to be simple, efficient and accurate.

A multi-dimensional Lagrangian algebraic slip mixture model was developed in this paper. This model was based on the idea of Shang [6,7]. It employed a mixture model to describe the multi-phase flows based on Eulerian model. The slip velocity, which can be developed from the dynamic equation of the dispersed phase based on Lagrangian model, was introduced to present the difference between dispersed and continuous phases. Owing to the Lagrangian model, the interfacial forces, such as buoyancy, drag force, lift force and virtual mass force etc., are enable to be involved in the multi-dimensional Lagrangian algebraic slip mixture model. It is therefore different from the traditional algebraic slip mixture model, which only considers the effects of gravity, centrifugal force and drag force, provided by FLUENT, CFX and other commercial software [1]. Through comparisons with experiments and other models on cylindrical and rectangle bubble columns, this model was validated.

2. Mathematical modeling

Considering a problem of turbulent multi-component multi-phase flow with one continuous phase and several dispersed phases, the time average conservation equations of mass, momentum and energy for the multi-dimensional Lagrangian algebraic slip mixture model as well as the turbulent kinetic energy equation and the turbulent kinetic energy transport equation can be written as the following [1,6–9].

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

$$\partial(\rho_m\mathbf{U}_m)/\partial t + \nabla\cdot(\rho_m\mathbf{U}_m\mathbf{U}_m) = -\nabla p + \rho_m\mathbf{g} + \nabla\cdot\left[(\mu_m+\mu_t)\left(\nabla\mathbf{U}_m + \nabla\mathbf{U}_m^T\right)\right] - \nabla\cdot\sum\alpha_i\rho_i\mathbf{U}_{im}\mathbf{U}_{im} \tag{2}$$

$$\partial(\rho_m h_m)/\partial t + \nabla\cdot(\rho_m\mathbf{U}_m h_m) = q + \nabla\cdot\left[\left(\frac{\mu_m}{Pr}+\frac{\mu_t}{Pr_t}\right)\nabla h_m\right] - \nabla\cdot\sum\alpha_k\rho_k h_k\mathbf{U}_{km}, \tag{3}$$

$$\partial(\rho_m k)/\partial t + \nabla\cdot(\rho_m\mathbf{U}_m k) = \nabla\cdot\left[\left(\mu_m+\frac{\mu_t}{\sigma_k}\right)\nabla k\right] + G - \rho_m\varepsilon, \tag{4}$$

$$\partial(\rho_m\varepsilon)/\partial t + \nabla\cdot(\rho_m\mathbf{U}_m\varepsilon) = \nabla\cdot\left[\left(\mu_m+\frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\right] + \frac{\varepsilon}{k}(C_1G - C_2\rho_m\varepsilon), \tag{5}$$

in which

$$\rho_m = \sum\alpha_i\rho_i, \tag{6}$$

$$\mu_m = \sum\alpha_i\mu_i, \tag{7}$$

$$\rho_m\mathbf{U}_m = \sum\alpha_i\rho_i\mathbf{U}_i, \tag{8}$$

$$\mathbf{U}_{im} = \mathbf{U}_i - \mathbf{U}_m, \tag{9}$$

$$G = \frac{1}{2}\mu_t\left[\nabla\mathbf{U}_m + (\nabla\mathbf{U}_m)^T\right]^2, \tag{10}$$

$$\mu_t = C_\mu\rho_m\frac{k^2}{\varepsilon}, \tag{11}$$