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Numerical simulation of turbulent solid–liquid two-phase flow and orientation of slender particles in a stirred tank

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Abstract

In this paper, turbulent solid–liquid two-phase flow involving slender particles in a tank stirred by standard Rushton turbines is simulated with two-fluid model using the improved inner–outer iterative method. Standard k–ε model is used to deal with turbulent flow. By comparison with the case of equivalent spherical particles, it is found that the flow field of slender particles is similar to that of spherical particles. The evolution of particle orientation as it follows the liquid flow in a stirred tank is modeled directly from the rigid slender rods revolution equation. Experiments about solid–liquid two-phase flow are also performed in a baffled tank using DPIV (digital particle image velocimetry). All simulation results are compared with experiments. The comparison between simulation and experiments confirms that the results are reliable. The good agreements between simulation and experiments verify the reliability of the methods employed in this paper. The influences of impeller speed on flow field and orientations are also investigated.

Keywords: Slender particle; Numerical simulation; DPIV; Flow field; Orientation; A stirred tank

1. Introduction

Agitated vessels are widely used in chemical, pharmaceutical and petroleum refinery industries for mixing and chemical reactions. Since flow in agitated vessels usually is turbulent, many turbulence models have been developed in the numerical research on agitated vessels, such as the standard k–ε turbulence model (isotropic turbulence model), algebraic stress model (ASM) (anisotropic turbulence model), etc. The treatment of impeller is one of the difficulties in simulating stirred tanks. Gosman et al. (1992) and Hou et al. (2001) used the 'black box' method to treat the impeller region with experimental data as boundary conditions. Following that, Ranade and Doment (1996) proposed snapshot approach. Brucato et al. (1998) proposed the inner–outer iterative method. Wang and Mao (2002a) improved the inner–outer iterative method.

Solid–liquid two-phase flow is often encountered in stirred tanks. The presence of solid particles makes the flow in stirred tanks more complicated. The most common two-phase flow models are followings (Zhou, 1993): continuous medium model, discrete particle model, pseudo-fluid model and the kinetic theory of granular flow. The continuous medium model is used widely in the field of two-phase flow. However, solid particles in stirred tanks are often simplified to be spherical particles. Spherical particles have been the focus of researchers for many years. Non-spherical particles are seldom involved.

Slender particles are significant to many process engineering industries. Owing to the special shape, research on slender particles has received more attention. Different from spherical particles, slender particles are orientation dependent. The orientation of slender particles plays a dominant

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role in its many applications. Therefore, it is necessary to study on orientation of slender particles. Jeffery's equation (1922) for the motion of an ellipsoidal particle in viscous medium form the basis of most of the researches performed in this field. For any two-dimensional homogeneous flow fields, the velocity gradient tensor can be specified as

$$u_{i,j} = \begin{pmatrix} \frac{\partial u_1}{\partial x_1} & \frac{\partial u_1}{\partial x_2} \\ \frac{\partial u_2}{\partial x_1} & \frac{\partial u_2}{\partial x_2} \end{pmatrix} = \begin{pmatrix} c & c_1 \\ c_2 & -c \end{pmatrix}.$$

For fibers with finite aspect ratios, the rotation equation can be expressed in the following form:

$$\overline{p}_i = (\Omega_{ij} + \lambda D_{ij}) p_j - \lambda p_i p_l p_k D_{lk}, \tag{1}$$

where Ω_{ij} and D_{ik} are vorticity and deformation rate tensors, respectively.

Based on Jeffery's equation, Givler et al. (1983), using local velocity gradient, solved the planar orientation angle along the streamlines with a finite element technique. Akbar and Altan (1992) expressed the fiber orientation using a unit vector. The orientation change was evaluated by considering the time rate of change of the unit vector. Then orientation of fibers in arbitrary two-dimensional homogeneous flow field could be analytically calculated. More quantitative analyses for predicting the orientation of slender particles in a variety of flow situations have been advanced in numerous studies. A wide range of analytical expressions describing the rotation of slender particles in mathematically tractable flow fields has been developed. However, most of them are limited to an arbitrary plane flow where the velocity components depend solely on the plane coordinates. Seldom simulation is on orientations in a three-dimensional flow field.

In this paper, both the three-dimensional two-fluid model and the improved inner–outer iterative method are employed to predict the turbulent flow field involving slender particles in an agitated vessel, stirred by standard Rushton turbines. The results are compared with experiments and that involving spherical particles with equal volume. At the same time, the orientations of slender particles in three-dimensional flow field, a stirred tank, is modeled. The orientations of slender particles are achieved directly from the evolution equation of rigid particle.

2. Flow model

2.1. Governing equations

Two-fluid model proposed by Ishii (1975) is used to simulate the flow field in a stirred tank, where both phases are assumed to coexist at every point in space in the form of interpenetrating continua. It is assumed that the fluid is incompressible and the interactions between particles are negligible. The force in the momentum exchange term mainly taken account is the drag force between fluid and particles.

In the cylindrical coordinate, continuity equations and momentum equations of liquid and solid are expressed as the followings.

$$(\rho_c \alpha_c u_{ci})_i = 0, \tag{2}$$

$$(\rho_d \alpha_d u_{di})_i = 0, \tag{3}$$

$$(\rho_c \alpha_c u_{ci} u_{cj})_j = -\alpha_c P_i + (\alpha_c \tau_{c,ij})_j + F_{cd,i} - \alpha_c \rho_c g_i, \tag{4}$$

$$(\rho_d \alpha_d u_{di} u_{dj})_j = -\alpha_d P_i + (\alpha_d \tau_{d,ij})_j - F_{cd,i} - \alpha_d \rho_d g_i, \tag{5}$$

$$\alpha_c + \alpha_d = 1, \tag{6}$$

where,

$$\tau_{c,ij} = \mu_c \left\{ u_{c,ji} + u_{c,ij} - \tfrac{2}{3}\delta_{ij} u_{c,kk} \right\},$$

$$\tau_{d,ij} = \mu_d \left\{ u_{d,ji} + u_{d,ij} - \tfrac{2}{3}\delta_{ij} u_{d,kk} \right\},$$

F_{cd} is drag force.

$$F_{cd} = \frac{S}{2} C_D \alpha_d (u_{d,i} - u_{c,i}) |u_{d,i} - u_{c,i}|. \tag{7}$$

Expression (8) (Fan et al., 2004) of drag coefficient C_D is obtained from experiments of slender particles, which is utilized to calculate the drag force between fluid and particles. The drag coefficient is based on the Reynolds number, the angle ϕ^* between the particle and the plane normal to velocity.

$$C_D \cos\phi^* = \frac{24}{Re}(0.006983 + 0.6224 Re^{-1.046}) \times \left(\frac{\rho_p}{\rho_l}\right)^{-1.537} (Ar^*)^{0.8524}, \tag{8}$$

where, Ar^* is the modified Archimedes number, $Ar^* = d_p^3(\rho_p - \rho_l)^2 g/\mu^2$. $Re = d_p(u_s - u_l)\rho_s/\mu_l$.

2.2. Turbulence model

Turbulent effects are modeled by standard k–ε model. In the cylindrical coordinate, the general equation for k and ε is written as

$$\frac{1}{r}\frac{\partial}{\partial r}(\rho_k r \alpha_k u_{kr}\phi) + \frac{1}{r}\frac{\partial}{\partial \theta}(\rho_k \alpha_k u_{k\theta}\phi) + \frac{\partial}{\partial z}(\rho_k \alpha_k u_{kz}\phi) = \frac{1}{r}\frac{\partial}{\partial r}\left(\alpha_k \mu_{k,\mathrm{eff}}\, r \frac{\partial \phi}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial \theta}\left(\frac{\alpha_k \mu_{k,\mathrm{eff}}}{r}\frac{\partial \phi}{\partial \theta}\right) + \frac{\partial}{\partial z}\left(\alpha_k \mu_{k,\mathrm{eff}} \frac{\partial \phi}{\partial z}\right) + S_\phi, \tag{9}$$