

Simulation of Solid Suspension in a Stirred Tank Using CFD-DEM Coupled Approach*

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Abstract Computational fluid dynamics-discrete element method (CFD-DEM) coupled approach was employed to simulate the solid suspension behavior in a Rushton stirred tank with consideration of transitional and rotational motions of millions of particles with complex interactions with liquid and the rotating impeller. The simulations were satisfactorily validated with experimental data in literature in terms of measured particle velocities in the tank. Influences of operating conditions and physical properties of particles (*i.e.*, particle diameter and density) on the two-phase flow field in the stirred tank involving particle distribution, particle velocity and vortex were studied. The wide distribution of particle angular velocity ranging from 0 to $10^5 \text{ r} \cdot \text{min}^{-1}$ is revealed. The Magnus force is comparable to the drag force during the particle movement in the tank. The strong particle rotation will generate extra shear force on the particles so that the particle morphology may be affected, especially in the bio-/polymer-product related processes. It can be concluded that the CFD-DEM coupled approach provides a theoretical way to understand the physics of particle movement in micro- to macro-scales in the solid suspension of a stirred tank.

Keywords stirred tank, solid suspension, particle rotation, computational fluid dynamics, discrete element method

1 INTRODUCTION

The suspension of solids in a stirred tank has drawn more and more attention owing to its wide applications in crystallization, cell cultivation, leach-precipitation, adsorption, pharmaceutical and food industries, *etc.* For a better understanding of the complex two-phase flow in the stirred tank, advanced laser instruments have been employed in the relevant researches. For example, laser Doppler velocimetry (LDV) was used to evaluate the liquid flow field and turbulence intensities in stirred vessels [1, 2]. Recently, the fluorescent particle image velocimetry (FPIV), a novel technique that combines PIV with digital image analysis, was applied for simultaneous velocity measurements in a stirred reactor [3]. For some opaque systems, computer automated radioactive particle tracking (CARPT) technique [4] was used to study the flow field of solids in dense liquid-solid suspensions and the electrical resistance tomography (ERT) technique was applied to measure the solid concentration profiles and the degree of mixing homogeneity [5]. However, the measurements generally focus on the liquid velocity and overall distribution of solids, while little attention has been paid to the movement of single particles and interactions between particles for the restrictions of measurement techniques.

The computational fluid dynamics (CFD) method has been applied to simulate the liquid-solid system in stirred tanks. Most of these simulations were based on the Eulerian-Eulerian model, with the solid phase considered as a continuous phase [6–12], so that the

behavior of single particles could not be disclosed. Another methodology for the CFD simulation of liquid-solid system is the Eulerian-Lagrangian model, *e.g.*, coupled with the CFD and discrete element method (CFD-DEM), where the particle-scale physics can be predicted. In this model, both particle-particle and particle-wall interactions are solved by Newtonian equations of motion, while the particle-liquid interaction is considered *via* the inter-phase exchange term. However, few researches employing the DEM method in a stirred tank have been reported [13–15] due to the complexity and difficulty in the CFD-DEM simulation. Recently, Sakai *et al.* [16] employed a Lagrangian-Lagrangian method for the simulation of a solid-liquid flow in a cylindrical tank without impellers.

In addition to the translational motion of particles, the rotation behavior is also important for its potential influence on the deformation and breakage of the particles, and even the heat transfer and the reaction inside them. For example, the Magnus force induced by particle rotation itself is an important factor affecting the particle movement [17]. In a stirred tank with an impeller rotating at high speed, the particle rotation is more complex due to frequent particle-impeller collisions as well as particle-particle contact and liquid-solid interaction. It is extremely difficult to measure the angular velocity of particle by the techniques available. As a consequence, the particle rotation has been seldom considered in literature.

This work aims to apply the CFD-DEM coupled approach to study the solid suspension behavior in a 3D stirred tank. Compared with the experimental

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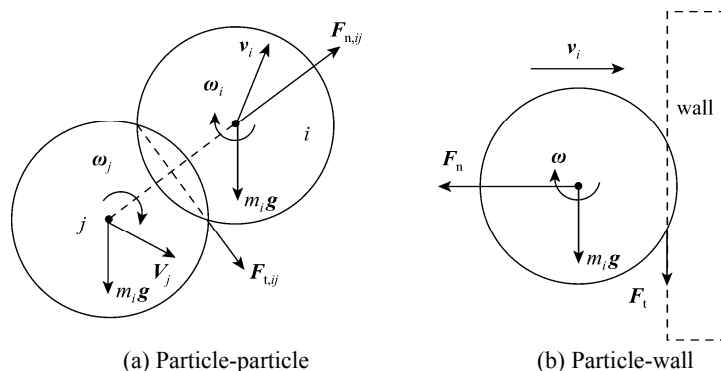


Figure 1 Forces acting on particles during collisions

measurements and CFD simulations based on Eulerian-Eulerian scheme, CFD-DEM simulation can provide more information for the flow field in the stirred tank, such as the concentration distribution, clustering, collision and rotation of particles.

2 MATHEMATICAL MODEL AND NUMERICAL SIMULATIONS

2.1 Mathematical model

2.1.1 Governing equations for liquid-phase flow

The governing equations for the liquid-phase flow consist of the continuity equation, the momentum equation and the turbulence model. The fluid is assumed to be incompressible. The equations are as follows.

Continuity equation:

$$\frac{\partial}{\partial t}(\alpha_l \rho_l) + \nabla(\alpha_l \rho_l \mathbf{u}) = 0 \quad (1)$$

Conservation equation of momentum:

$$\frac{\partial}{\partial t}(\alpha_l \rho_l \mathbf{u}) + \nabla(\alpha_l \rho_l \mathbf{u} \mathbf{u}) = -\nabla p + \nabla(\alpha_l \mu_l \nabla \mathbf{u}) + \rho_l \alpha_l \mathbf{g} - \mathbf{S} \quad (2)$$

where α is the volume fraction of relevant phase, $\mathbf{S}$ is the source term from the particle-liquid interaction, and subscript 'l' refers to liquid.

Realizable k - ε turbulence model [18]:

$$\frac{\partial}{\partial t}(\alpha_l \rho_l k) + \nabla(\alpha_l \rho_l \mathbf{u} k) = \nabla \left(\alpha_l \left(\mu_l + \frac{\mu_t}{\sigma_k} \right) \nabla k \right) + \alpha_l G_k - \alpha_l \rho_l \varepsilon \quad (3)$$

$$\frac{\partial}{\partial t}(\alpha_l \rho_l \varepsilon) + \nabla(\alpha_l \rho_l \mathbf{u} \varepsilon) = \nabla \left(\alpha_l \left(\mu_l + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right) + \alpha_l \rho_l \left(C_1 S \varepsilon - C_2 \frac{\varepsilon^2}{k + \sqrt{\nu \varepsilon}} \right) \quad (4)$$

$$\mu_t = \rho_l C_\mu \frac{k^2}{\varepsilon} \quad (5)$$

where parameters $C_1 = 1.44$, $C_2 = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1.0$ and $\sigma_\varepsilon = 1.2$.

2.1.2 Discrete element model for the motion of particles

The transitional motion of a particle depends on the sum of forces acting on it, while the rotational motion is controlled by contact torques.

$$m_i \frac{d\mathbf{v}_i}{dt} = m_i \mathbf{g} + \sum_{j=1}^{n_i} (\mathbf{F}_{n,ij} + \mathbf{F}_{t,ij}) + \mathbf{F}_{D,i} + \mathbf{F}_{M,i} + \mathbf{F}_{b,i} \quad (6)$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{n_i} (\mathbf{T}_{t,ij} + \mathbf{T}_{r,ij}) \quad (7)$$

Besides the liquid-solid interactions, drag force $\mathbf{F}_D$ and Magnus force $\mathbf{F}_M$, the forces acting on particle stem from particle-particle, particle-wall and particle-impeller collisions, which are illustrated in Figs. 1 and 2.

Particle-particle collisions

The contact forces and torques between two spherical particles are based on the classical Hertz-Mindlin model [19–21]. The normal force $\mathbf{F}_{n,ij}$ between particles i and j is

$$\mathbf{F}_{n,ij} = \frac{4}{3} Y^* \sqrt{R^*} \delta_{n,ij}^{3/2} - \mathbf{F}_{n,ij}^d \quad (8)$$

$$\mathbf{F}_{n,ij}^d = -2 \sqrt{\frac{5}{6}} \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \sqrt{S_{n,ij} m^*} \mathbf{v}_n \quad (9)$$

$$S_{n,ij} = 2Y^* \sqrt{R^*} \delta_{n,ij} \quad (10)$$

where Y^* is the equivalent Young's modulus, m^* is the particle mass, R^* is the equivalent radius, $\delta_{n,ij}$ is the normal overlap, $S_{n,ij}$ is the normal stiffness, $\mathbf{v}_n$ is the normal component of the relative velocity, and e is the coefficient of restitution.

The tangential force $\mathbf{F}_{t,ij}$ depends on the tangential overlap $\delta_{t,ij}$ and the tangential stiffness $S_{t,ij}$, and limited by Coulomb friction $\mu_s \mathbf{F}_{n,ij}$, where μ_s is the coefficient of static friction and G^* is the shear modulus.

$$\mathbf{F}_{t,ij} = -\delta_{t,ij} S_{t,ij} - \mathbf{F}_{t,ij}^d \quad (11)$$

$$\mathbf{F}_{t,ij}^d = -2\sqrt{\frac{5}{6}} \frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \sqrt{S_{t,ij} m^*} \mathbf{v}_t \quad (12)$$

$$S_{t,ij} = 8G^* \sqrt{R^* \delta_{n,ij}} \quad (13)$$

The torques generated by the forces can be written as

$$\mathbf{T}_{t,ij} = L_{ij} \mathbf{n}_{ij} \times \mathbf{F}_{t,ij} \quad (14)$$

$$\mathbf{T}_{r,ij} = -\mu_t L_{ij} |\mathbf{F}_{n,ij}| \frac{\boldsymbol{\omega}_{ij}}{|\boldsymbol{\omega}_{ij}|} \quad (15)$$

where L_{ij} is the distance from the center of particle i to the contact plane with particle j , $\mathbf{n}_{ij}$ represents the normal unit vector between two contacted particles, and $\boldsymbol{\omega}_{ij}$ is the angular velocity vector of the object at the contact point.

Particle-wall and particle-impeller collisions

During a particle-wall collision, the forces and the torques on the particle are similar to those in particle-particle collisions, as shown in Eq. (8) to Eq. (15). For dilute particles in the system, the reverse effects of particles on the tank wall and impeller are ignored in the simulation.

Different from the particle-wall collision, the particle-impeller collision is more complex owing to the impeller rotation. The impeller blades move along the tangential direction and affect the tangential behavior of particles, so only the velocity on the tangential direction is displayed. As shown in Fig. 2, at time t_1 , the particle moves towards the impeller blade, and collides with it at time t_2 with the tangential velocity of $\mathbf{v}_{t_2}$. Then the tangential velocity of particle gradually decreases to 0 at t_3 . After that, the particle bounces back to the opposite tangential direction and the collision finishes at time t_5 . At each discrete

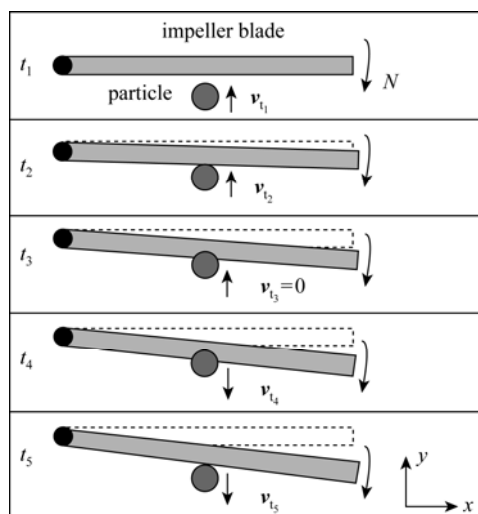


Figure 2 A sketch of particle-impeller collision

time-step during the collision, the forces and the torques acting on particles are calculated based on Eq. (8) to Eq. (15).

The time-step for DEM simulation is 1.5×10^{-6} s, and the maximum impeller movement at its tip in a DEM time-step is about 5×10^{-6} m. This value is much less than the particle diameter, so the simulation precision can be ensured with the physical model.

2.1.3 Interaction between liquid and particles

The momentum sink $\mathbf{S}$ is a volumetric summation of the forces between the liquid and particles. $\mathbf{F}_p$ is the force exerting on the fluid in a CFD mesh cell and V_{cell} is the cell volume. In this work, buoyant force $\mathbf{F}_b$, drag force $\mathbf{F}_D$ and the Magnus force $\mathbf{F}_M$ caused by the particle rotation are considered. Thus, $\mathbf{S}$ is calculated as

$$\mathbf{S} = \frac{\sum_i^n \mathbf{F}_p}{V_{\text{cell}}} = \frac{\sum_i^n (\mathbf{F}_{D,i} + \mathbf{F}_{M,i} + \mathbf{F}_{b,i})}{V_{\text{cell}}} \quad (16)$$

$$\mathbf{F}_b = -\frac{1}{6} \pi d_p^3 \rho_l \mathbf{g} \quad (17)$$

Drag force

For the drag force $\mathbf{F}_D$, the Di Felice drag model [22] is used. It adds a correction term to the free stream drag model to take into account the effects of neighboring particles on the drag force. The model is formulated as

$$\mathbf{F}_D = \mathbf{F}_{D0} \alpha_p^{-(\beta-1)} \quad (18)$$

$$\mathbf{F}_{D0} = \frac{\pi}{8} \rho_l C_D d_p^2 \alpha_p^2 |\mathbf{u} - \mathbf{v}| (\mathbf{u} - \mathbf{v}) \quad (19)$$

$$\beta = 3.7 - 0.65 \exp \left[-\left(1.5 - \lg Re_p\right)^2 / 2 \right] \quad (20)$$

$$C_D = \begin{cases} \frac{24}{Re_p} & Re_p \leq 1 \\ \left(0.63 + \frac{4.8}{Re_p^{0.5}}\right)^2 & Re_p > 1 \end{cases} \quad (21)$$

$$Re_p = \frac{\alpha_p \rho_l d_p |\mathbf{u} - \mathbf{v}|}{\mu_l} \quad (22)$$

Magnus force

The Magnus effect is induced when a spinning object moves in a fluid, and the Magnus force perpendicular to the line of motion is created by a whirlpool of fluid around itself. The Magnus force $\mathbf{F}_M$ is calculated as [23, 24]

$$\mathbf{F}_M = 0.125 \pi d_p^3 \rho_l \frac{Re_1}{Re_2} C_L \left[(0.5 \boldsymbol{\omega}_l - \boldsymbol{\omega}_p) \times (\mathbf{u} - \mathbf{v}) \right] \quad (23)$$

$$C_L = 0.45 + \left(\frac{Re_1}{Re_2} - 0.45 \right) \exp(-0.05684 Re_1^{0.3} Re_2^{0.4}) \quad (24)$$

$$Re_1 = \frac{|\mathbf{u} - \mathbf{v}|}{\mu_l} d_p \quad (25)$$

$$Re_2 = \frac{|0.5\omega_l - \omega_p|}{\mu_l} d_p^2 \quad (26)$$

where ω_l is the local vorticity of liquid and ω_p is the angular velocity of particle.

2.2 Configuration of stirred tank

The experimental work in a Rushton stirred tank using the CARPT technique [4] is used for the validation of numerical simulations. The simulated system is a flat-bottomed Rushton turbine tank with diameter $T=0.2$ m and equal liquid height (H). The tank is equipped with four vertical baffles of $T/10$ in width and $T/125$ in thickness. Both the impeller diameter and impeller bottom clearance are $T/3$. The simulations are conducted in a 3D domain. The vessel geometry is meshed with 564309 cells as shown in Fig. 3 (a). To investigate the particle behavior in local regions, three planes (30° , 45° and 60°) between the baffles and two planes (10° and -10°) around the baffles are considered, as shown in Fig. 3 (b).

2.3 Numerical method

In the CFD-DEM coupled approach, FLUENT 6.3.26 and EDEM 2.2.1 are successfully coupled: the equations of liquid flow are solved using FLUENT, while the equations of DEM model are solved by EDEM. To simulate the rotational motion of the impeller, the algorithm of multiple reference frames is applied. The regions around the impeller are simulated in a rotating frame of reference, while the other regions in the tank are applied with a stationary frame of reference. The no slip condition is applied at the tank wall and the impeller, and the free slip condition is

adopted for the liquid surface. In each case, the single-phase flow is simulated without particles for 5 seconds to reach the steady state. Then particles are introduced to the whole tank randomly, and the time releasing the first particle is considered as $t=0$. From $t=0$ to 0.01 s, the particles are continuously released to the whole tank uniformly.

2.4 Computational conditions

The DEM time-step τ_{DEM} is usually determined by the Rayleigh time step. It is judged that all the energy is transferred by the Rayleigh waves [25]. As a result, the Rayleigh time step, defined as the time for a DEM simulation of a quasi-static particulate collection in which the coordination number (total number of contacts per particle) for each particle remains above 1, can be calculated as [26]

$$\tau_R = 0.5\pi d_p \left(\frac{\rho_p}{G^*} \right)^{1/2} / (0.1631\sigma + 0.8766) \quad (27)$$

In this work, τ_{DEM} is set as 1.5×10^{-6} s ($40\% \tau_R$) to ensure good performance for particle simulation. The CFD time-step is set as 5.0×10^{-5} s (about $30 \tau_{DEM}$). The continuum model of liquid is solved by the SIM-PLC method and its momentum equations are solved by the second-order implicit time integration. The explicit time integration method is used to solve the translational and rotational motions of particles in DEM simulation. The physical properties of dilute particles and the liquid employed in the simulation and the simulation parameters, if not mentioned in particular, are the same as those listed in Table 1.

3 RESULTS AND DISCUSSION

3.1 Validation of CFD-DEM simulations

The CFD-DEM simulations are validated by

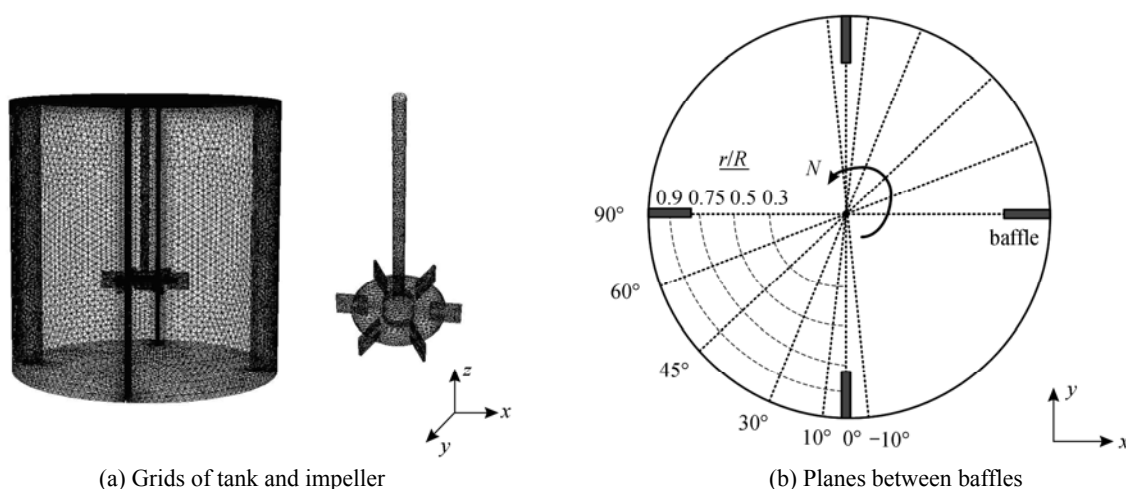
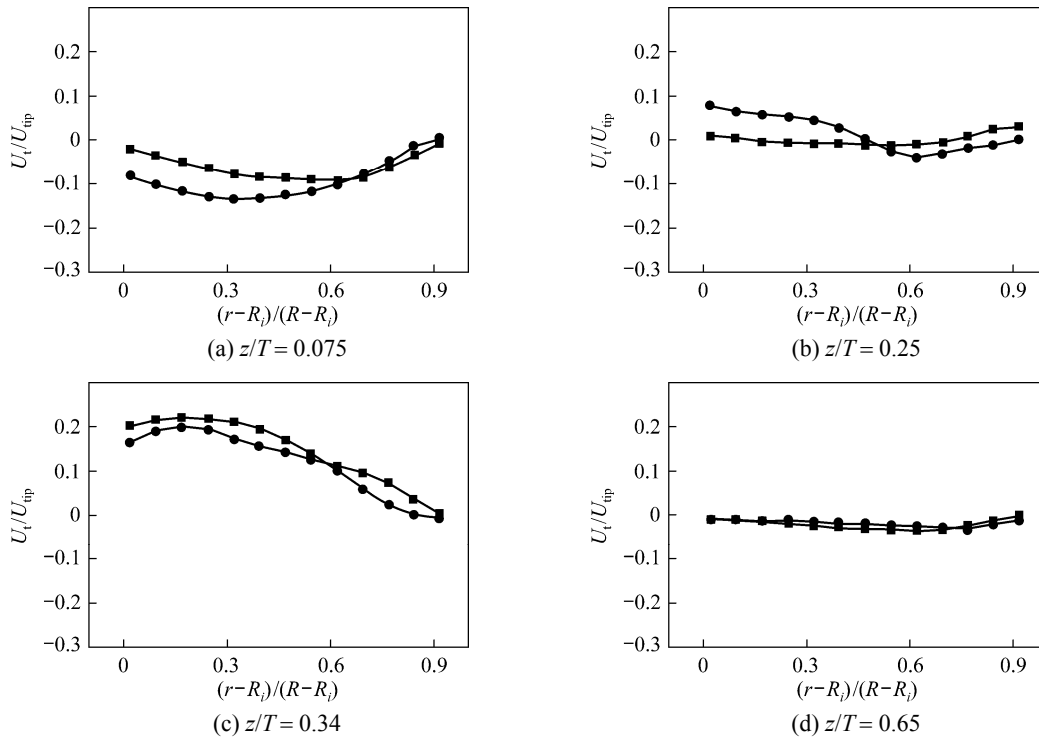


Figure 3 An overview of the stirred tank adopted for the CFD-DEM simulation

Table 1 Physical properties and simulation parameters

Particle diameter (d_p)/mm	Particle density (ρ_p)/kg·m ⁻³	Liquid density (ρ)/kg·m ⁻³	Liquid viscosity (μ)/Pa·s	Number of particles	Young's modulus (Y)/GPa	Shear modulus (G^*) /GPa
0.3	2500	1000	0.001	4000000	0.1 [27, 28]	0.04 ($Y^*/G^* = 2 + 2\sigma$)
Poisons ratio (σ)	Coefficient of restitution (e)	Static friction coefficient (μ_s)	Rolling friction coefficient (μ_r)	CFD time-step (τ_{CFD})/s	DEM time-step (τ_{DEM})/s	
0.25 [27, 28]	0.9 [27, 28]	0.3 [27, 28]	0.1 [26]	5×10^{-5}	1.5×10^{-6}	

**Figure 4** Radial profiles of solid radial velocity in the stirred tank (solid holdup of 1% at 1000 r·min⁻¹)

■ simulation; ● experiment

experimental measurements [4] in terms of the profiles of particle velocity. The comparisons of radial profiles of radial velocity, tangential velocity and axial velocity of particles are shown in Figs. 4–6, where all the velocity data are normalized by the impeller tip speed U_{tip} . Four axial planes, $z/T = 0.075$ (tank bottom), $z/T = 0.25$ (below the impeller), $z/T = 0.34$ (impeller height) and $z/T = 0.65$ (midway between impeller and liquid surface), are chosen to validate the simulation results. The numerical simulations are in reasonably good agreement with the experimental measurements [4], though some errors can be justified. The radial, tangential and axial velocity profiles of particles are dependent on the spatial positions in the stirred tank, especially affected by the relative position to the impeller, since the impeller generates the flow field in the liquid-solid stirred tank.

3.2 Particle distribution in the stirred tank

3.2.1 Axial distribution of particles

Figure 7 shows the transient liquid flow pattern

and spatial distribution of particles at different axial planes. The particle clustering phenomenon is more evident at the tank bottom than at the top. At the axial plane $z/T = 0.05$ near the tank bottom, particles move along the liquid streamlines. In particular, the heterogeneous flow structure and low axial velocity in the bottom region lead to high-density clusters of particles. At the plane $z/T = 0.35$, particles move along different rings, due to the strong turbulence and high liquid velocity in this region. At $z/T = 0.8$ near the tank surface, particles are more uniformly dispersed, due to the low axial and radial velocities. The 2D field data at these planes all illustrate the dependence of particle distribution on the liquid flow field.

The particle concentration C in specified region is characterized by the number of particles per unit volume. Hence the value C can be defined based on the comparison to the whole tank C_{av} (6.4×10^8 particles·m⁻³):

$$\frac{C}{C_{\text{av}}} = \frac{NP_{\text{local}}/V_{\text{local}}}{NP_{\text{total}}/V} = \frac{NP_{\text{local}} \times V}{NP_{\text{total}} \times V_{\text{local}}} \quad (28)$$

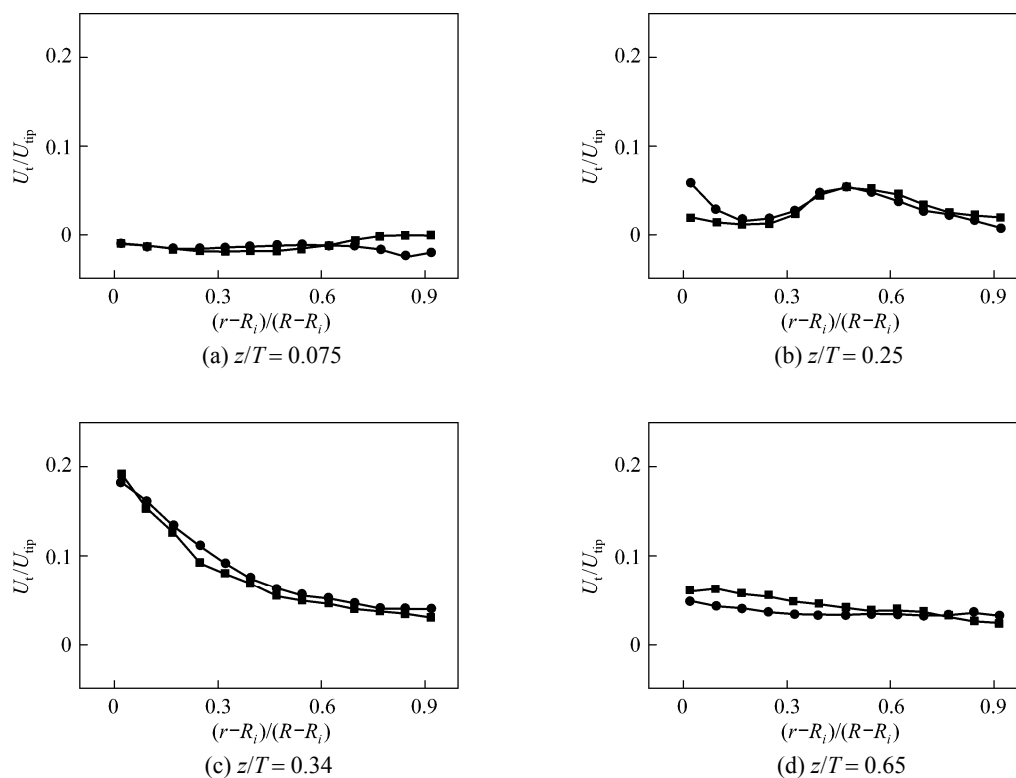


Figure 5 Radial profiles of solid tangential velocity in the stirred tank (solid holdup of 1% at $1000 \text{ r} \cdot \text{min}^{-1}$)
 ■ simulation; ● experiment

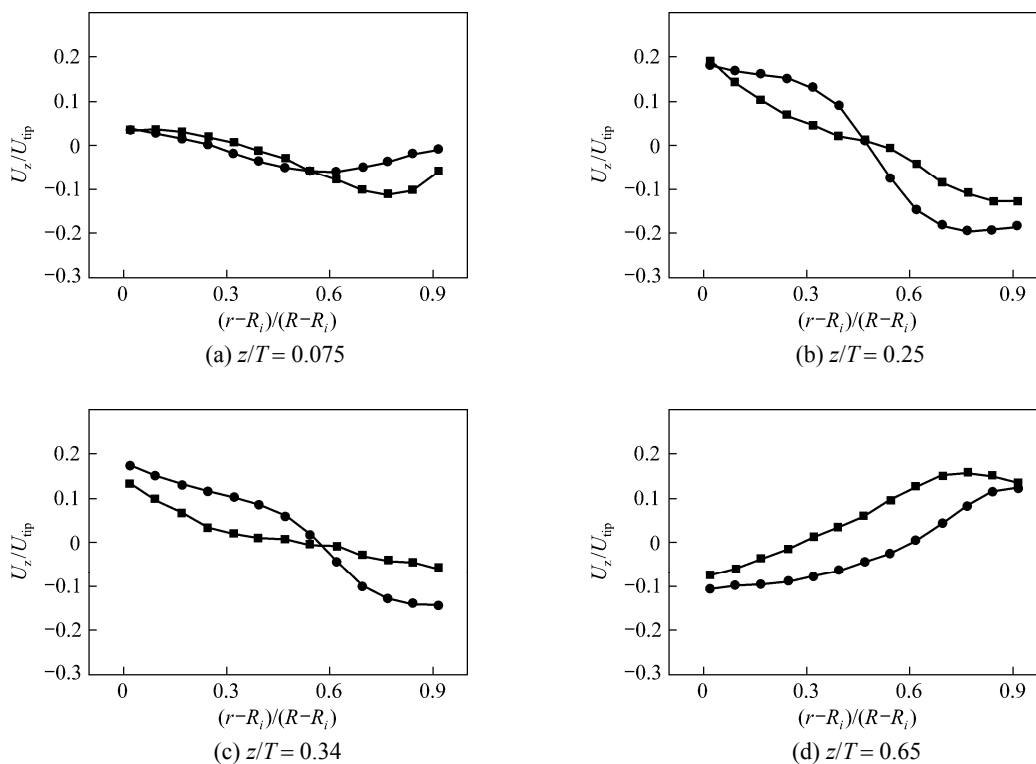


Figure 6 Radial profiles of solid axial velocity in the stirred tank (solid holdup of 1% at $1000 \text{ r} \cdot \text{min}^{-1}$)
 ■ simulation; ● experiment

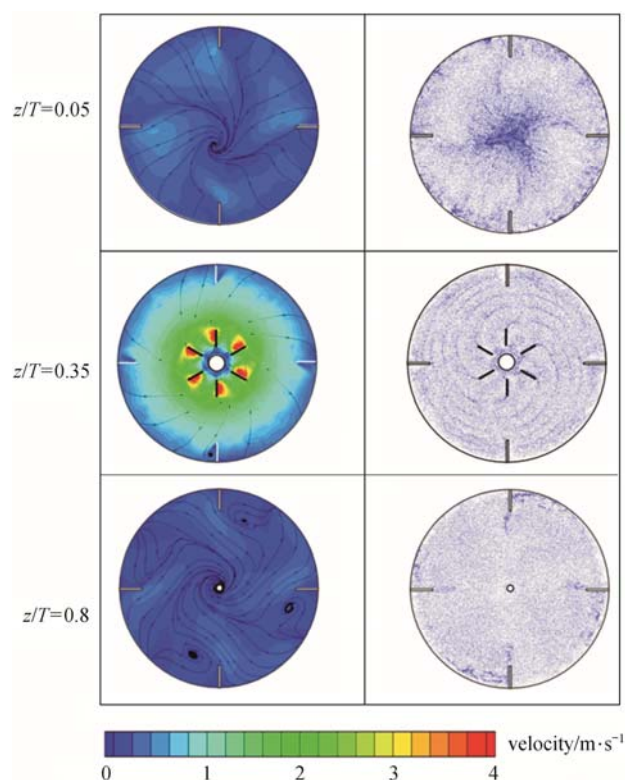


Figure 7 Snapshots of liquid flow pattern and particle concentration distribution at different axial planes in the stirred tank ($t = 2$ s)

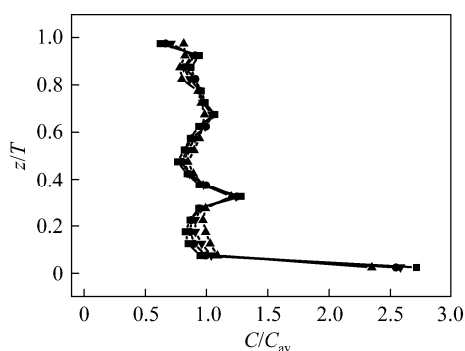


Figure 8 Axial profiles of solid concentrations in the stirred tank at $1000 \text{ r} \cdot \text{min}^{-1}$

■ 1 s; ● 1.5 s; ▲ 2 s; ▼ 1–2 s

The time-averaged particle concentration from 1 s to 2 s is measured by 100 sampling points, as shown below

$$\left(\frac{C}{C_{av}} \right)_{1-2s} = \frac{(NP_{local})_{1.01s} + (NP_{local})_{1.02s} + \dots + (NP_{local})_{2.00s}}{100 \times NP_{total}} \frac{V}{V_{local}} \quad (29)$$

The axial profiles of particle concentration at 1, 1.5, and 2 s and the time-averaged one are shown in

Fig. 8. The particles are not uniformly distributed throughout the tank while the particle concentration above the impeller ($z/T = 0.33$) is relatively low. At the impeller height, there is a sudden increase of C/C_{av} due to the clustering of particles caused by the low axial velocity between vortices below and above the impeller. The maximum particle concentration appears near the tank bottom at low radial and axial velocities, as indicated in Section 3.1. The time-averaged particle concentration profile is similar to the transient ones, showing steady statistics from 1 s to 2 s. Hence, all the time-averaged parameters in the later discussion are based on the averaged values from 1 s to 2 s.

3.2.2 Particle distributions at different vertical cross-sections

Figure 9 shows the transient liquid flow pattern and particle distribution at the vertical planes of three angles (30° , 45° , and 60° as indicated in Fig. 3). The particle clusters locate mainly in three regions. One is right below the impeller, where the liquid velocity magnitude is relatively small; one is at the impeller plane, where the liquid axial velocity is lower between liquid vortices; and one is at the axial position of $z/T = 0.7$, where the liquid axial velocity at the vortex boundary is small. It can be concluded that the particle distribution depends on the liquid velocity (or vortex) distribution and more particles are easy to reside around the liquid vortices.

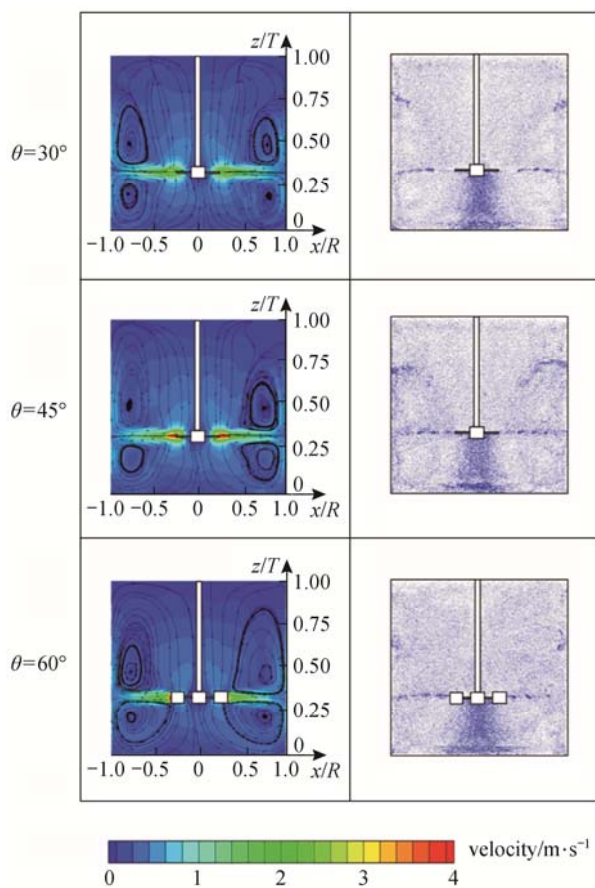


Figure 9 Snapshots of liquid flow pattern and particle concentration distribution at different planes between the baffles ($t = 2$ s)

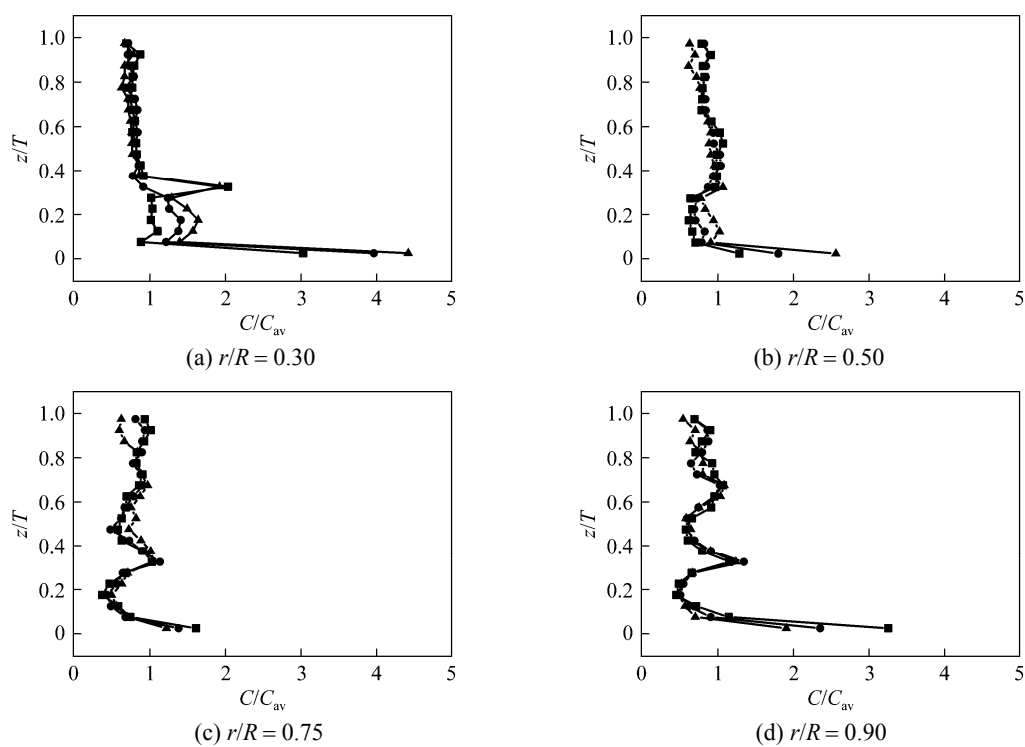


Figure 10 Axial and radial profiles of phase-averaged particle concentrations on the planes between two baffles
 ■ 30°; ● 45°; ▲ 60°

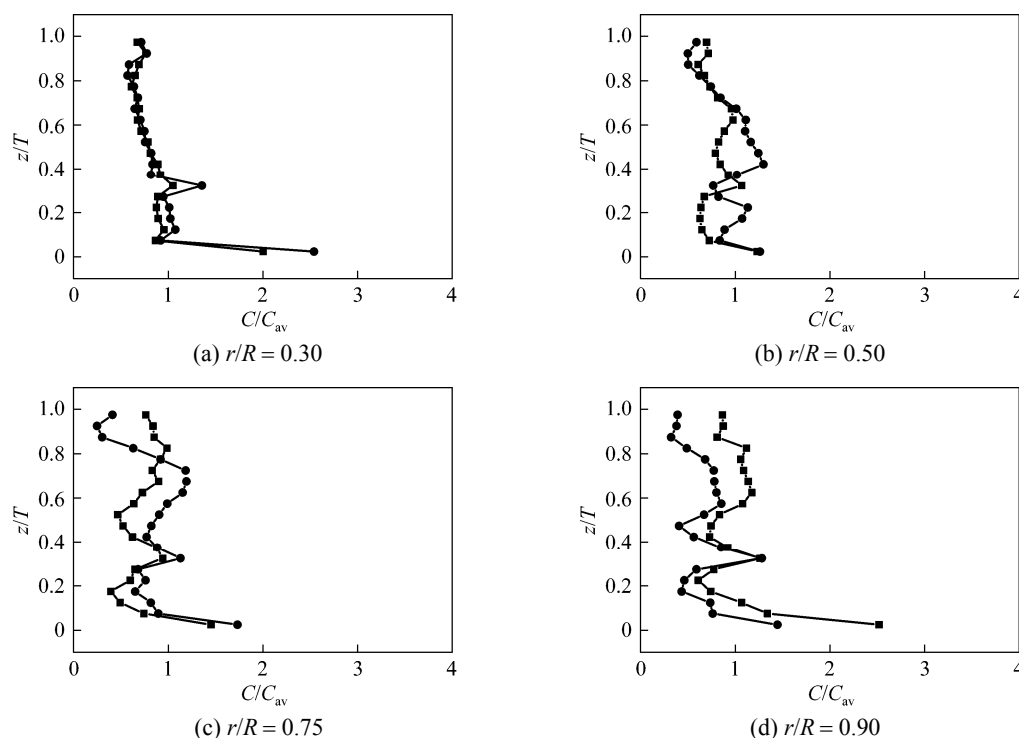


Figure 11 Particle concentrations at the front (10°) and back (-10°) of the baffle
 ■ 10° ; ● -10°

Figure 10 illustrates the particle concentration at local planes. At the radial position $r/R=0.3$ and axial position $z/T>0.33$, the particle concentrations at the three observation angles are nearly the same. However, at the impeller height $z/T=0.33$, C/C_{av} gets a sharp increase at 60° and 30° , while the change at 45° is slight. At $z/T<0.33$, C/C_{av} drops sharply at 60° and increases slowly at 45° and 30° . At the radial position $r/R=0.5$, the particle concentrations above the impeller show consistent behavior at the three angles, while the profiles of particle concentration are more complex at $r/R=0.75$ and $r/R=0.9$. For all the observation angles, the highest concentration is 4.4 near the tank bottom at 30° due to the low velocities in axial and radial directions.

3.2.3 Particle distribution around baffles

In order to investigate the effect of baffles on the particle distribution, the particle concentrations at the front (10°) and back (-10°) of the baffle are considered, as shown in Fig. 11. At $r/R=0.3$ with the same axial height, there is no distinct difference in particle concentrations between the two planes. At $r/R=0.5$, the concentration at the back plane is higher than the front one at $z/T<0.7$, while there is no significant difference at $z/T>0.7$. At $r/R=0.75$, the particle concentration of the back plane is lower with $z/T>0.7$, but the tendency is reversed with $z/T<0.7$. At $r/R=0.9$, the concentration at the front plane is higher than that at the back plane for all the axial heights. The comparison shows that concentration C at the front plane gradually exceeds the back one with the increase of r/R .

3.3 Particle collisions

Similar to the definition of particle concentration, the particle collision frequency is expressed by the number of collisions (NC). Particle collisions involve particle-particle, particle-impeller and particle-wall interactions. Fig. 12 shows the particle collision rate normalized by the averaged value NC_{av} (2.61×10^{10} collisions $\cdot m^{-3} \cdot s^{-1}$) in the whole tank. The particle collision rate NC/NC_{av} near the tank bottom is about 5.3, while the value near the impeller height is 2.2. In other regions, NC/NC_{av} is less than 0.3. It is clear that particle collisions mainly take place in two regions, *i.e.*, the tank bottom and the impeller height.

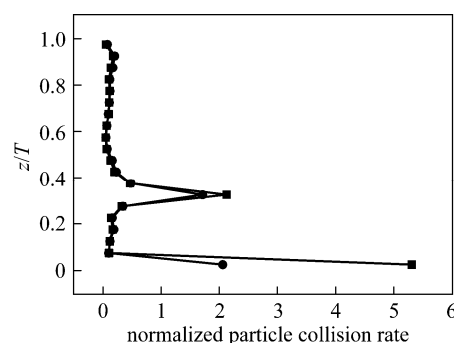


Figure 12 Radial profiles of particle collision rate ($t=1-2$ s)
 ■ NC/NC_{av} ; ● $r_c/r_{c,av}$

To eliminate the effect of particle concentration on the total number of collisions, the collision rate r_c is defined in terms of NC/C , and the value relative to the averaged one $r_{c,av}$ is defined as

$$\frac{r_c}{r_{c,av}} = \frac{NC}{NC_{av}} \bigg/ \frac{C}{C_{av}} \quad (30)$$

The maximum $r_c/r_{c,av}$ is 2.1 near the tank bottom, that is, higher particle concentration contributes to more frequent collisions. At the impeller height, the collision rate is 1.8, due to the high particle concentration and fast impeller motion. In other regions with low C , the collision rate $r_c/r_{c,av}$ is less than 0.5, showing the dependence of collision on particle concentration.

3.4 Particle rotations

Generally, the Magnus force (F_M) caused by particle rotation is ignored in CFD simulations since it is negligible compared to the drag force (F_D). However, in the simulation of solid suspension in stirred tanks, the ratio F_M/F_D should be considered since many particles rotate with high angular velocities. At the impeller speed $N = 1000 \text{ r} \cdot \text{min}^{-1}$, the time-averaged F_M/F_D for all particles is about 0.14. Statistics of all the particles give the averaged F_M/F_D in different scales: 0.0019 for $\omega_p = 0-1 \text{ r} \cdot \text{min}^{-1}$, 0.021 for $\omega_p = 1-10 \text{ r} \cdot \text{min}^{-1}$, 0.054 for $\omega_p = 10-100 \text{ r} \cdot \text{min}^{-1}$, 0.12 for $\omega_p = 100-1000 \text{ r} \cdot \text{min}^{-1}$, 0.34 for $\omega_p = 1000-10000 \text{ r} \cdot \text{min}^{-1}$ and 1.20 for $\omega_p = 10000-100000 \text{ r} \cdot \text{min}^{-1}$. This indicates that F_M/F_D increases with angular velocity. For particles with ω_p lower than $100 \text{ r} \cdot \text{min}^{-1}$, the Magnus force is much lower than the drag force, but it is in the same order of magnitude as the drag force when ω_p is ranged from 100 to $10000 \text{ r} \cdot \text{min}^{-1}$. For particles with $\omega_p > 10000 \text{ r} \cdot \text{min}^{-1}$, the averaged Magnus force even exceeds the drag force. Hence, the Magnus force cannot be ignored in a stirred system with high impeller rotation speed.

The tendencies of curves in Fig. 13 are similar to the axial distributions of particle concentration. The

maximum F_M/F_D and ω_p appear at the impeller height owing to higher particle concentration and more frequent particle-impeller collisions. Another region with relatively high F_M/F_D and ω_p is near the tank bottom, because of the high particle concentration and collision rate, as explained in Section 3.3. However, the value near the tank bottom is less than that at the impeller height, since the collisions between particles at the tank bottom are weaker.

To illustrate the particle angular velocity distribution along the axial height z/T in more details, we define P as the local probability of particle angular velocity and P_{av} as the probability in the whole tank. The profiles of P/P_{av} in Fig. 14 (a) show that all the particles with ω_p of $0-1 \text{ r} \cdot \text{min}^{-1}$ are at the tank bottom. Many of the particles near the tank bottom have the angular velocity magnitude of $1000-10000 \text{ r} \cdot \text{min}^{-1}$ because of the frequent collisions between the particles and the tank bottom. Owing to the intense collisions between the impeller and the particles, most of the particles with angular velocity magnitude of $10000-100000 \text{ r} \cdot \text{min}^{-1}$ are near the impeller height. In addition, the particles around the impeller region seldom have angular velocity less than $100 \text{ r} \cdot \text{min}^{-1}$. It is concluded that the high particle angular velocity is attributed to the strong collisions between the impeller and particles.

3.5 Factors affecting particle distribution and rotational motions

3.5.1 Impeller speed

When the impeller speed decreases to $800 \text{ r} \cdot \text{min}^{-1}$ and $600 \text{ r} \cdot \text{min}^{-1}$, many of the particles settle to the bottom of the tank, with averaged particle angular velocity decreasing to $503 \text{ r} \cdot \text{min}^{-1}$ and $391 \text{ r} \cdot \text{min}^{-1}$ respectively. This indicates significant effect of impeller speed on particle rotations. The axial profiles of particle angular velocities at impeller speeds of $800 \text{ r} \cdot \text{min}^{-1}$ and $600 \text{ r} \cdot \text{min}^{-1}$, illustrated as the red and blue lines in Fig. 13 (a), present consistent behavior as that at $N = 1000 \text{ r} \cdot \text{min}^{-1}$, with the maximum angular velocities decreasing sharply. The decrease of maximum

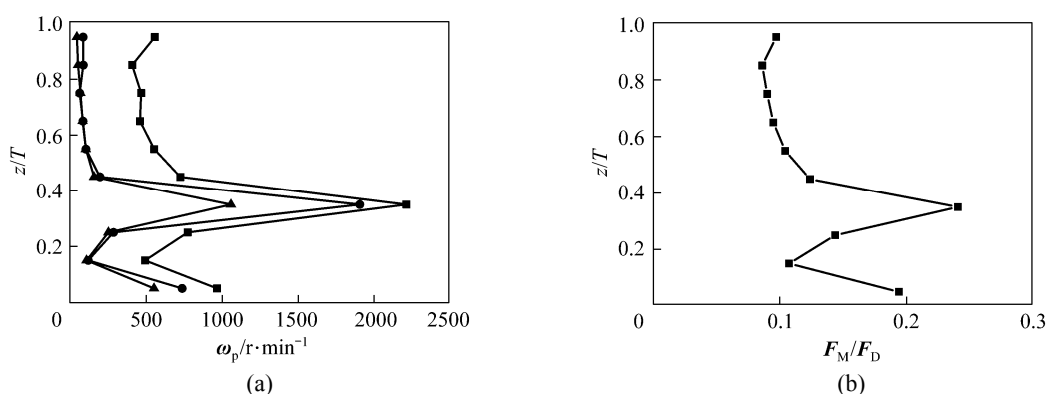


Figure 13 Axial distributions of particle angular velocity (a) and ratio of Magnus force to drag force (b)

■ $N = 1000 \text{ r} \cdot \text{min}^{-1}$; ● $N = 800 \text{ r} \cdot \text{min}^{-1}$; ▲ $N = 600 \text{ r} \cdot \text{min}^{-1}$

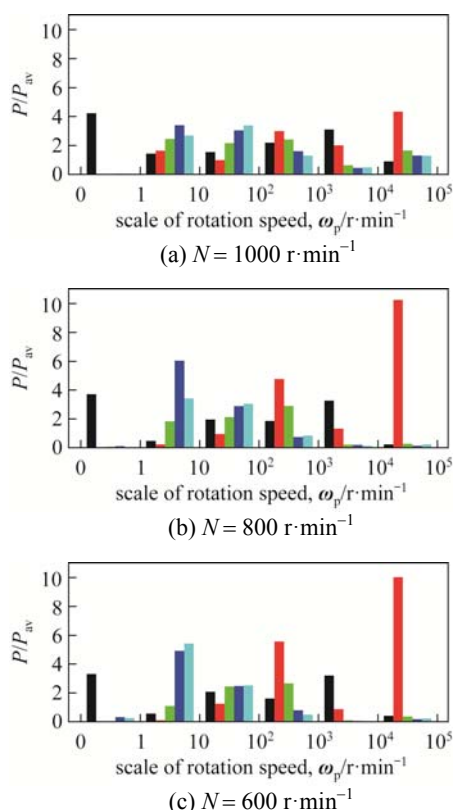


Figure 14 Probability distributions of particle angular velocity at different axial zones

z/T : ■ 0.0–0.2; ■ 0.2–0.4; ■ 0.4–0.6; ■ 0.6–0.8; ■ 0.8–1.0

ω_p is owing to the less intense particle collisions caused by lower particle transitional velocities, since

the stirring speed is reduced.

The probability distributions of ω_p at $N=800$ $\text{r}\cdot\text{min}^{-1}$ and 600 $\text{r}\cdot\text{min}^{-1}$ shown in Fig. 14 (b)–14 (c) are similar to each other while they are quite different from that at $N=1000$ $\text{r}\cdot\text{min}^{-1}$. One distinct difference is the peak values of P/P_{av} at $\omega_p=10^4$ – 10^5 $\text{r}\cdot\text{min}^{-1}$, showing that almost all of the particles with high angular velocities are at the impeller height when the impeller speed is low. This indicates the more evident contribution of particle-impeller interactions to the high particle angular velocities at low stirring rates. Another difference is that at $N=600$ $\text{r}\cdot\text{min}^{-1}$, particles with ω_p as low as 0 – 1 $\text{r}\cdot\text{min}^{-1}$ appear in the above half part of the tank, probably because at such low impeller speed, the liquid velocity is so low that the particle rotations are quite slow at this region.

3.5.2 Particle diameter

Particles with diameter between 100 μm and 250 μm are considered to investigate the effect of particle diameter on the spatial distributions of particles. The operating conditions are the same as that shown in Table 1 with the number of particles changed to 10000 , and the impeller speed is 1000 $\text{r}\cdot\text{min}^{-1}$. The axial profiles of particle concentration with different particle diameters illustrated in Fig. 15 (a) show that the particles with smaller diameters distribute more uniformly throughout the tank, since they are easy to move along liquid streamlines and disperse uniformly. Moreover, particle concentration C near the tank surface is higher than the averaged concentration C_{av} for smaller particles. There is no significant difference among the axial profiles of particle angular velocity with various particle diameters, as shown in Fig. 15 (b). Axial profiles above the impeller are nearly the same. The differences can be justified mainly in two regions: the impeller

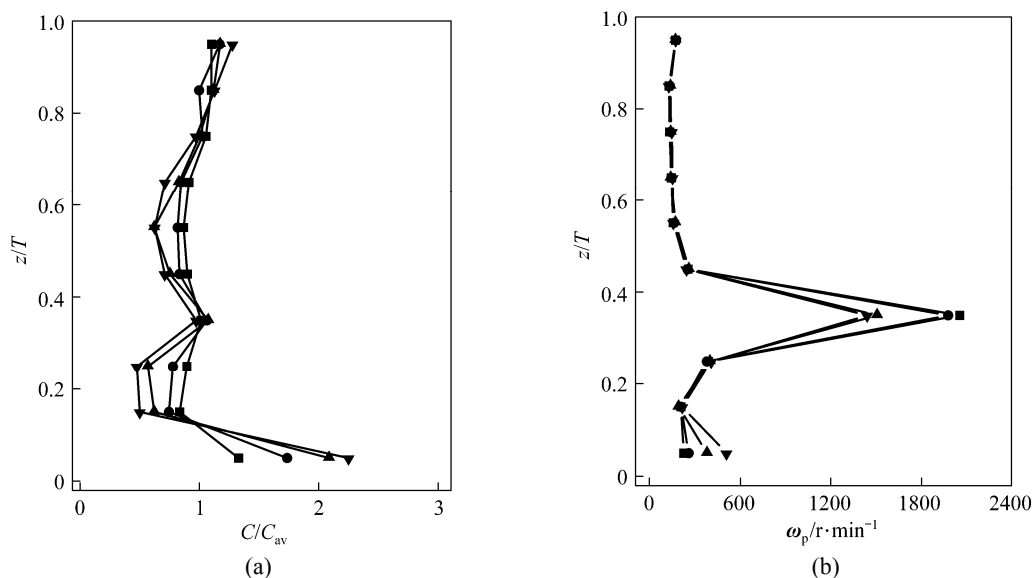


Figure 15 Axial profiles of particle concentration (a) and particle angular velocity (b) with different particle diameters at impeller speed of $N=1000$ $\text{r}\cdot\text{min}^{-1}$

$d_p/\mu\text{m}$: ■ 100; ● 150; ▲ 200; ▼ 250

height and the tank bottom. At the impeller height, smaller particles have higher angular velocities because of relatively higher torques generated by particle-impeller interactions; while, at the tank bottom, smaller particles have lower angular velocities owing to the less frequent particle-particle collisions since the particle concentration is lower.

3.5.3 Particle density

Particles with diameter of 300 μm and different densities of 800, 1000, 1200 and 1500 $\text{kg}\cdot\text{m}^{-3}$ are considered. Other conditions are the same as that mentioned above. Fig. 16 shows that particle density has certain effect on particle concentration distribution, especially at the top and bottom of the tank. Particle concentration at the tank bottom is lower while concentration near the liquid surface becomes higher with decreasing particle density, since particles at low density tend to float near the liquid surface owing to relatively high buoyancy.

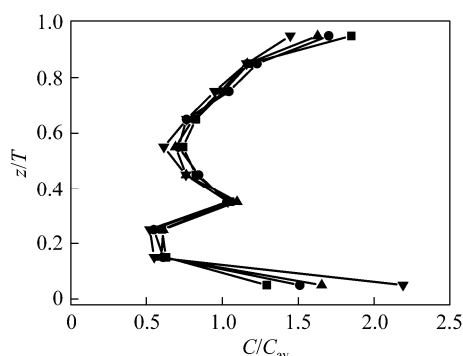


Figure 16 Axial distributions of solid concentrations with different particle densities at impeller speed of $N = 1000 \text{ r}\cdot\text{min}^{-1}$ particle density/ $\text{kg}\cdot\text{m}^{-3}$: ■ 800; ● 1000; ▲ 1200; ▼ 1500

5 CONCLUSIONS

Solid suspension in a stirred tank was investigated by the numerical simulation based on CFD-DEM coupled approach. With the distinct advantage of the Eulerian-Lagrangian modeling scheme, the particle-scale physics, including particle motion, particle collision and particle rotation behavior, can be disclosed dynamically in detail. The meso- and macro-scale statistics such as the spatial distribution of particle velocity and concentration in Eulerian space were successfully calculated. The following conclusions can be drawn from the present work.

(1) CFD-DEM simulations are satisfactory, validated by the experimental particle velocities in radial, axial and tangential directions in literature.

(2) The simulation results clearly show the clustering phenomenon of particles in the liquid-solid stirred system. Particle clusters easily form near the tank bottom for the low axial velocity. At the plane below and above the impeller, distinct particle clustering phenomena also appear due to the vortices.

(3) The particle collision rate is determined by the local distribution of particle concentration. Higher particle concentration contributes to more frequent particle collisions.

(4) The particle angular velocity obtained by the CFD-DEM simulation has a wide distribution ranging from 0 to $10^5 \text{ r}\cdot\text{min}^{-1}$. For strong particle rotation, the Magnus force on the particle cannot be ignored since it has the same order of magnitude as the drag force when ω_p ranges from 100 to 10000 $\text{r}\cdot\text{min}^{-1}$ and even exceeds the drag force when $\omega_p > 10000 \text{ r}\cdot\text{min}^{-1}$. The particle rotation and its wide distribution in speed may introduce uncertain effect on some processes related to the quality of particle product, the lifetime of cells in a bioreactor due to the extra shear, etc. This topic is rarely explored either in the academia or in the industry.

(5) The effects of operating conditions and physical properties of particles on particle concentration distribution and angular velocity can be predicted reasonably using the CFD-DEM model.

NOMENCLATURE

C	particle concentration in specified region, m^{-3}
C_{av}	average particle concentration in the whole tank, m^{-3}
C_D	drag coefficient
d_p	particle diameter, m
e	coefficient of restitution
$F_{b,i}$	buoyant force on the particle i , N
F_{D0}	drag force, N
$F_{D,i}$	drag force on particle i , N
$F_{M,i}$	Magnus force on particle i , N
$F_{n,ij}$	normal contact force between particles i and j , N
$F_{n,ij}^d$	normal damping force between particles i and j , N
F_p	force exerting on the fluid in a CFD mesh cell, N
$F_{t,ij}$	tangential contact force between particles i and j , N
$F_{t,ij}^d$	tangential damping force between particles i and j , N
G^*	shear modulus, GPa
G_k	generation of turbulence kinetic energy due to the mean velocity gradient, J
g	acceleration of gravity, $\text{N}\cdot\text{kg}^{-1}$
H	liquid height, m
I_i	moment of inertia of particle i , $\text{kg}\cdot\text{m}^2$
k	turbulence kinetic energy, J
L_{ij}	distance from the center of particle i to the contact plane with particle j , m
m_i	mass of particle i , kg
m^*	equivalent particle mass, kg
N	impeller speed, $\text{r}\cdot\text{min}^{-1}$
NC	number of particle collisions
NP_{local}	particle number in specified region
NP_{total}	particle number in the whole tank
$\mathbf{n}_{ij}$	normal unit vector between contacted particles i and j
P	probability distribution of particle angular velocity
p	pressure, Pa
R	tank diameter, m
R^*	equivalent radius, m
Re_p	particle Reynolds number
r	radial position in the tank, m
r_c	particle collision rate, s^{-1}
r_{av}	average particle collision rate in the whole tank, s^{-1}
S	source term in the momentum equation, $\text{N}\cdot\text{m}^{-3}$
$S_{n,ij}$	normal stiffness between particles i and j , $\text{N}\cdot\text{m}^{-1}$
$S_{t,ij}$	tangential stiffness between particles i and j , $\text{N}\cdot\text{m}^{-1}$
T	tank height, m

$T_{t,ij}$	torque between particles i and j generated by tangential forces, N·m
$T_{r,ij}$	torque between particles i and j generated by radial forces, N·m
t	time, s
U_r	radial velocity of solid, $\text{m}\cdot\text{s}^{-1}$
U_t	tangential velocity of solid, $\text{m}\cdot\text{s}^{-1}$
U_z	axial velocity of solid, $\text{m}\cdot\text{s}^{-1}$
U_{tip}	tip speed of impeller, $\text{m}\cdot\text{s}^{-1}$
$\mathbf{u}$	velocity vector, $\text{m}\cdot\text{s}^{-1}$
V	volume of tank, m^3
V_{cell}	volume of CFD mesh cell, m^3
V_{local}	volume of specified region, m^3
$\mathbf{v}_i$	translational velocity of particle i , $\text{m}\cdot\text{s}^{-1}$
$\mathbf{v}_n$	normal component of the relative velocity between two contacted particles, $\text{m}\cdot\text{s}^{-1}$
$\mathbf{v}_t$	tangential component of the relative velocity between two contacted particles, $\text{m}\cdot\text{s}^{-1}$
Y^*	equivalent Young's modulus, GPa
z	height of axial plane, m
α_l	volume fraction of liquid phase
α_p	volume fraction of particles
$\delta_{n,ij}$	normal overlap between particles i and j , m
$\delta_{t,ij}$	tangential overlap between particles i and j , m
ε	turbulent dissipation rate, W
μ_l	liquid viscosity, Pa·s
μ_r	coefficient of rolling friction
μ_s	coefficient of static friction
μ_t	turbulent viscosity, Pa·s
ρ_l	density of liquid phase, $\text{kg}\cdot\text{m}^{-3}$
ρ_p	particle density, $\text{kg}\cdot\text{m}^{-3}$
σ	Poisson's ratio
σ_k	turbulent Prandtl number for k
σ_ε	turbulent Prandtl number for ε
τ_{CFD}	CFD time step, s
τ_{DEM}	DEM time step, s
τ_R	Rayleigh time step, s
$\mathbf{v}$	kinematic viscosity, $\text{m}^2\cdot\text{s}^{-1}$
$\boldsymbol{\omega}_i$	angular velocity of particle i , $\text{rad}\cdot\text{s}^{-1}$
$\boldsymbol{\omega}_{ij}$	angular velocity vector of the object at the contact plane of particles i and j , $\text{rad}\cdot\text{s}^{-1}$
ω_l	local vorticity of liquid, $\text{rad}\cdot\text{s}^{-1}$
ω_p	angular velocity of particle, $\text{rad}\cdot\text{s}^{-1}$

Subscripts

av	average
c	collision
D	drag
i	particle i
j	particle j
k	turbulence kinetic energy
l	liquid
M	Magnus
n	normal
p	particle
R	Rayleigh
r	radial
t	tangential
z	axial
μ	viscosity

REFERENCES

- Virdung, T., Rasmuson, A., "Measurements of continuous phase velocities in solid-liquid flow at elevated concentrations in a stirred vessel using LDV", *Chem. Eng. Res. Des.*, **85** (A2), 193–200 (2007).
- Nouri, J.M., Whitelaw, J.H., "Particle velocity characteristics of dilute to moderately dense flows in stirred reactors", *Int. J. Multiphase Flow*, **18** (1), 21–33 (1992).
- Unadkat, H., Rielly, C.D., Hargrave, G.K., Nagy, Z.K., "Application of fluorescent PIV and digital image analysis to measure turbulence properties of solid-liquid stirred suspensions", *Chem. Eng. Res. Des.*, **87** (4), 133–142 (2009).
- Guha, D., Ramachandran, P.A., Dudukovic, M.P., "Flow field of suspended solids in a stirred tank reactor by Lagrangian tracking", *Chem. Eng. Sci.*, **62** (22), 6143–6154 (2007).
- Hosseini, S., Patel, D., Ein-Mozaffari, F., Mehrvar, M., "Study of solid-liquid mixing in agitated tanks through electrical resistance tomography", *Chem. Eng. Sci.*, **65** (4), 1374–1384 (2010).
- Gosman, A.D., Issa, R.I., Lekakou, C., Looney, M.K., Politis, S., "Multidimensional modelling of turbulent two-phase flow in stirred vessels", *AIChE J.*, **38** (12), 1946–1956 (1992).
- Micale, G., Rizzuti, F., Brucato, A., "CFD simulation of particle suspension height in stirred vessels", *Chem. Eng. Res. Des.*, **82** (9), 1204–1213 (2004).
- Fan, L., Mao, Z.S., Yang, C., Wang, Y.D., "Numerical simulation of laminar solid-liquid two-phase flow in stirred tank", *Chem. Eng. Commun.*, **194** (3), 291–308 (2007).
- Kasat, G.R., Khopkar, A.R., Ranade, V.V., Pandit, A.B., "CFD simulation of liquid-phase mixing in solid-liquid stirred reactor", *Chem. Eng. Sci.*, **63** (15), 3877–3885 (2008).
- Shan, X.G., Yu, G.Z., Yang, C., Mao, Z.S., Zhang, W.G., "Numerical simulation of liquid-solid flow in an unbaffled stirred tank with a pitched-blade turbine downflow", *Ind. Eng. Chem. Res.*, **47** (9), 2926–2940 (2008).
- Wang, G., Zhou, S., Yang, F., Chen, S., "A CFD study of an up- and a down-pumping PBT impeller in solid-liquid stirred tank", *Adv. Mater. Res.*, **354-355**, 696–700 (2011).
- Feng, X., Li, X.Y., Cheng, J.C., Yang, C., Mao, Z.S., "Numerical simulation of solid-liquid turbulent flow in a stirred tank with a two-phase explicit algebraic stress model", *Chem. Eng. Sci.*, **82** (1), 272–284 (2012).
- Decker, S., Sommerfeld, M., "Calculation of particles suspension in agitated vessels with the Euler-Lagrange approach", *ICHEME Symp. Series*, **140**, 71–82 (1996).
- Derkson, J.J., "Numerical simulation of solids suspension in a stirred tank", *AIChE J.*, **49** (11), 2700–2714 (2003).
- Srinivasa, T., Jayanti, S., "An Eulerian/Lagrangian study of solid suspension in stirred tanks", *AIChE J.*, **53** (9), 2461–2469 (2007).
- Sakai, M., Shigeto, Y., Sun, X., Aoki, T., Saito, T., Xiong, J., Koshizuka, S., "Lagrangian-Lagrangian modeling for a solid-liquid flow in a cylindrical tank", *Chem. Eng. J.*, **200-202** (15), 663–672 (2012).
- Wu, X., Wang, Q., Luo, Z., Fang, M., Cen, K., "Theoretical and experimental investigations on particle rotation speed in CFB riser", *Chem. Eng. Sci.*, **63** (16), 3979–3987 (2008).
- Shih, T.H., Shabbir, W.W., Yang, Z., Zhu, J., "A new k - ε eddy-viscosity model for high Reynolds number turbulent flows model development and validation", *Computers & Fluids*, **24** (3), 227–238 (1995).
- Mindlin, R.D., "Compliance of elastic bodies in contact", *J. Appl. Mech.*, **16** (3), 259–268 (1949).
- Mindlin, R.D., Deresiewicz, H., "Elastic spheres in contact under varying oblique forces", *J. Appl. Mech.*, **20** (3), 327–344 (1953).
- Langston, P.A., Tüzün, U., Heyes, D.M., "Discrete element simulation of granular flow in 2D and 3D hoppers: Dependence of discharge rate and wall stress on particle interactions", *Chem. Eng. Sci.*, **50** (6), 967–987 (1995).
- Di Felice, R., "The voidage function for fluid-particle interaction systems", *Int. J. Multiphase Flow*, **20** (1), 153–159 (1994).
- Mei, R., "An approximate expression for the shear lift force on a spherical particle at finite Reynolds numbers", *Int. J. Multiphase Flow*, **18** (1), 145–147 (1992).
- Oesterleé, B., Bui Dinh, T., "Experiments on the lift of a spinning sphere in a range of intermediate Reynolds numbers", *Exp. Fluids*, **25** (1), 16–22 (1998).
- Thomton, C., Randall, C.W., "Applications of theoretical contact mechanics to solid particle system simulation", In: *Micromechanics of Granular Materials*, Elsevier, Amsterdam, 133–142 (1988).
- Li, Y., Xu, Y., Thomton, C., "A comparison of discrete element simulations and experiments for 'sandpiles' composed of spherical particles", *Powder Technol.*, **160** (3), 219–228 (2005).
- Alberto, D.R., Francesco, P.D.M., "Homogeneous and bubbling fluidization regimes in DEM-CFD simulations: Hydrodynamic stability of gas and liquid fluidized beds", *Chem. Eng. Sci.*, **62** (1-2), 116–130 (2007).
- Alberto, D.R., Francesco, P.D.M., Rossella, G., Brunello, F., "DEM simulation of the mixing equilibrium in fluidized beds of two solids differing in density", *Powder Technol.*, **184** (2), 214–223 (2008).