**Lagrangian simulation of particle properties and stirring condition effects on solid particle distributions in stirred tanks with different size**

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**Highlights**

* The vertical distribution of particle concentration was calculated using CFD-DEM.
* A parameter was found to ascertain the dispersion state in the tank.
* An equation was proposed to predict particle concentration at the vertical height.

**1. Introduction**

Solid–liquid mixing is widely used in crystallizers and chemical reactors with catalysis. In these processes, some difficulties occur by which solid particles aggregate and collide with stirring blades. Particle collision causes particle breakage and abrasion. Furthermore, when scaling up to the scale to industrial equipment, the particle dispersion state usually becomes insufficient. It is important to qualify the solid particle concentration distribution in the tank and to ascertain the dispersion state to solve these problems. However, it is difficult to measure the detailed particle concentration in the tank under many conditions. Therefore, for this study, Euler–Lagrangian simulations were performed with various particle diameters, particle densities, impeller speeds, impeller diameters, and tank diameters to qualify the vertical distribution of solid particle concentrations in the vessel. We also identified the factors affecting the dispersion state.

**2. Analytical method**

The Euler–Lagrangian approach, which tracks all particle motion, was used. Turbulent flow in the vessel was represented by Large Eddy Simulation. The particle–particle and particle – solid surfaces interactions were modeled using distinct element method. Simulations were conducted using Computational Fluid Dynamics software (FLUENT 18.0; ANSYS Inc.). The simulated system was a flat-bottom cylindrical vessel with four baffles and a six-blade paddle impeller. Tank diameter *T* was changed from 10 cm to 30 cm with geometrical similarity. The diameter was equal to liquid height *H*. The impeller diameter *D* was *T*/2. Blade width *b* was *T*/10. The impeller bottom clearance was *T*/3. The impeller speed *N* was 4.0–6.0 s-1. The fluid was presumed to be water. The solid particle density was changed from 1011 to 2500 kg/m3. The diameter of the 5000 particles varied: 100–400 µm. The tank interior was divided into 50 zones in the vertical direction. The particle concentration in each zone at height *C*i and the particle concentration of the entire tank *C*av were calculated. The standard deviation of particle concentration $σ\_{c}$ was calculated using *C*i and *C*av. The time-averaged values of $σ\_{c}$, $σ\_{c,av}$ were used as particle dispersion state evaluation indexes for the vessel.

**3. Results and Discussion**

Fig. 1 portrays the relation between ${σ\_{c,av}}/{C\_{av}}$ and ${u\_{t}}/{(N D^{0.8})}$ . Here, *u*t, *N*, and *D* respectively represent the terminal velocity of a single particle, impeller speed, and impeller diameter. Results from Fig. 1 show that ${σ\_{c,av}}/{C\_{av}}$ is correlated with the value of ${u\_{t}}/{(N D^{0.8})}$, irrespective of the particle properties, impeller speed, and vessel size. Furthermore, results show that the particles are well dispersed in the tank in the range of at ${u\_{t}}/{ND^{0.8}}$ < 0.03, and that most of the particles are deposited on the bottom in the range of ${u\_{t}}/{ND^{0.8}}$ > 0.06. These results demonstrate that using the scale-up factor of ‘*ND*0.8 = constant’ enables the change of dispersion state in the small tank to be reproduced when scaling up to the large tank. The vertical component of fluid velocity near the bottom is presented in Fig. 2. The y-axis shows $\overbar{v\_{z}}$ /(*ND*0.8), which was of the time-averaged value $\overbar{v\_{z}}$ of the vertical velocity near the tank bottom (*z*/*H* = 0.1) along the tank centre section divided by $N D^{0.8}$. The figure shows that the distributions of vertical fluid velocities have nearly the same profile, irrespective of the impeller speed or tank diameter. The uniformity of particle concentration in the vertical direction, ${σ\_{c,av}}/{C\_{av}}$ can be arranged according to the ratio of $u\_{t}$ to $ND^{0.8}$, probably because the distribution of $\overbar{v\_{z}}$/(*ND*0.8) near the bottom, which is the fluid flow suspending the particles, shows a similar profile.

Fig. 3 portrays the vertical distribution of particle concentration in the range of 0.03 < ${u\_{t}}/{(ND^{0.8})}$ < 0.06. This figure shows that the dispersion state of the particles varies greatly in this range. Because ${σ\_{c,av}}/{C\_{av}}$ depends strongly on ${u\_{t}}/{(ND^{0.8})}$, the particle concentration *C*/*C*av is normalized by ${u\_{t}}/{(ND^{0.8})}$ in that range, as portrayed in Fig. 4. Results show that, by multiplying ${u\_{t}}/{ND^{0.8}}$, it is integrated roughly into one line. Fitting was performed using an exponential function for 0.03 < ${u\_{t}}/{(ND^{0.8})}$ < 0.06. The following equation was found.

(*C*/*C*av) *u*t/(*ND*0.8) = 0.0297 + 0.0427 exp (−7.12 *z*/*H*) (1)

Using equation (1), the particle concentration at the vertical height can be predicted at ±30 % irrespective of the particle property, impeller speed, and vessel size.



**Fig. 1** Relation between **Fig. 2** Distribution of $\overbar{v\_{z}}$/*ND*0.8 **Fig. 3** Particle concentration **Fig. 4** Particle concentration

*u*t/*ND*0.8 and ${σ\_{c,av}}/{C\_{av}}$ at *z*/*H* =0.1 in *r*-*z* plane at 0.03 < ${u\_{t}}/{ND^{0.8}}$ < 0.06 normalized by ${u\_{t}}/{ND^{0.8}}$

**4. Conclusions**

The vertical distribution of the particle concentration in the stirred vessel was analyzed using Euler–Lagrangian method. Results show that the deviation of particle concentration is correlated with the ratio of terminal velocity of single particle *u*t to *ND*0.8. In addition, in the range of 0.03 < ${u\_{t}}/{(ND^{0.8})}$ <0.06, an equation (Eq. (1)) was established as capable of predicting the particle concentration distribution in the vertical direction based on ${u\_{t}}/{(ND^{0.8})}$.

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