VOL. 48
NO. 5
M A Y
2 0 1 5

JCEJ

JOURNAL OF CHEMICAL ENGINEERING OF JAPAN

[VOL. 48, NO. 5, MAY 2015]

Special Issue for 4th Asian Conference on Mixing 2013 (ACOM4)

The Society of
Chemical Engineers,
Japan

JCEJAQ 48(5)
327-394(2015)
ISSN 0021-9592

Models and Applications for Simulating Turbulent Solid–Liquid Suspensions in Stirred Tanks

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Keywords: Solid–Liquid Suspension, Stirred Tank, Simulation, Eulerian, Lagrangian

Solid–liquid suspensions in stirred tanks are common unit operations in many process industries. The complex flow characteristics of these systems, such as two-phase turbulence and interphase interaction, make the corresponding numerical simulations complicated and challenging. This paper presents a review of models dealing with the continuous and discrete phases of solid–liquid suspensions and summarizes the applications for simulating related flow phenomena, including velocity and turbulence components, solids concentration, just-suspended speed, cloud height, optimization of geometrical parameters, and particle shape and type. Perspectives concerning different modeling approaches are presented, and the Eulerian–Lagrangian approach with resolved particles is highlighted to address the underlying suspension mechanisms in stirred tanks.

Introduction

Solid–liquid suspensions are important unit operations in many process industries such as chemical and pharmaceutical engineering, crystallization, polymerization, and water treatment. With the rapid development of computational fluid dynamics (CFD) and high performance computing, numerical approaches for simulating solid–liquid suspensions in stirred tanks have continued to burgeon.

Generally, the modeling of two-phase particulate flows falls into one of two categories, i.e., the Eulerian–Eulerian (E–E) or the Eulerian–Lagrangian (E–L) approach. In the E–E approach, the two phases are considered to be interpenetrating continua and the governing equations representing the conservation of mass and momentum are solved for both phases on an Eulerian grid. In the E–L approach, the conventional governing equations are utilized to solve the flow field of the continuous phase, and the discrete phase must be analyzed by tracking all the particles (Derksen, 2003) or clusters of particles (parcels) (Derksen *et al.*, 2008) as they move through the flow domain.

A plethora of experimental data on solid–liquid suspensions in stirred tanks has been amassed (Kasat and Pandit, 2005), including data on the two-phase velocity and turbulence components, solids concentration, just-suspended speed, and cloud height. Such data can be utilized to verify various CFD models. Valid CFD models are prospectively useful as aids for the design and optimization of stirred tanks containing solid–liquid suspensions.

In this paper, we summarize the models and applications for simulating solid–liquid suspensions in stirred tanks. Perspectives on the various simulation approaches are presented, and calculations employing the Eulerian–Lagrangian approach with resolved particles are introduced with emphasis on the current developments in this topic.

The current paper complements the recent review by Kaminoyama (2014) that discusses visualization of flow phenomena in agitated slurry vessels. The focus of the latter paper is on the use of CFD (as well as Electrical Resistance Tomography (ERT)) for elucidation of flow structures in optically inaccessible slurry systems, whereas the emphasis of the present paper is on the level of realism that can be achieved in CFD simulations of stirred solid–liquid suspensions and how this level relates to various computational approaches for turbulent multiphase flow.

1. Models for Continuous Phase

The continuum method for the fluid phase has been applied to both the E–E and E–L approaches. In order to simulate turbulent continuous single-phase flows, three approaches are usually utilized: Reynolds averaged Navier–Stokes (RANS) simulation, large eddy simulation (LES), and direct numerical simulation (DNS). These approaches and their applications to stirred tanks have been reviewed in detail by Sommerfeld and Decker (2004), Van den Akker (2010), and Joshi *et al.* (2011a, 2011b). The present section focuses on the models for simulating the influence of the discrete phase on the continuous phase in comparison with single-phase flows.

Received on January 31, 2014; accepted on April 25, 2014
DOI: 10.1252/jcej.14we056
Presented at 4th Asian Conference on Mixing (ACOM4) at Beijing, September 2013
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1.1 Reynolds averaged Navier–Stokes simulation

RANS-type models are most widely used for dealing with the turbulent continuous phase in simulations of solid–liquid suspensions in stirred tanks. For E–E simulations, the volume fraction of each phase is introduced in the continuity and momentum equations. The turbulent dispersion of the volume fraction is sometimes included in the continuity equations, and the turbulent Schmidt number is set to 0.8 (Tamburini *et al.*, 2009). The underlying theory of this dispersion term has not been sufficiently explored and validated in the literature, and numerical simulations including this term clearly do not give rise to improved results (Tamburini *et al.*, 2011).

Phase interaction forces such as drag, added mass, lift, history, and stress gradient forces are usually included in the momentum equations of the two phases in E–E simulations. Therefore, such simulations belong to the class of two-way coupling approaches (Gosman *et al.*, 1992). Ljungqvist and Rasmuson (2001) reported that the drag force is the dominating force acting on the particles, while the added mass force, the lift force, and the turbulent dispersion force have very little effect on the calculated slip velocities. Derksen (2003) estimated that the ratio of the lift (Magnus and/or Saffman force) to drag forces could reach 0.8 to 1 in the impeller region, which indicates the significance of the lift force. The latter paper also estimated the value of the Basset history force and proposed that the Basset force could be neglected in comparison with the drag force. In the literature, forces other than the drag force are usually ignored for the sake of simplicity (Murthy *et al.*, 2007; Tamburini *et al.*, 2011).

Several drag force correlations (Clift *et al.*, 1978; Magelli *et al.*, 1990; Brucato *et al.*, 1998; Pinelli *et al.*, 2001; Khopkar *et al.*, 2006) have been summarized (Ochieng and Onyango, 2010; Sardeshpande and Ranade, 2012). Wadnerkar *et al.* (2012) compared the effect of four drag models and found that the results from the modified Brucato drag model (Khopkar *et al.*, 2006) were in reasonable agreement with the experimental data. Sardeshpande *et al.* (2011) found that the coefficient in the Brucato drag model was dependent on the particle diameter, solids loading, particle Reynolds number, and prevailing turbulence. Both the Brucato and the modified Brucato drag models overestimated the axial slip velocity in the impeller region. Similar results for drag models were obtained by Ochieng and Onyango (2008). Thus, further study is required to clarify the overall effect of drag models on the flow hydrodynamics in stirred tanks.

To model the turbulent stress in solid–liquid systems, three different extensions of the standard k–ε model, namely the "for each phase" model, the "mixture" or "homogeneous" model, and the "dispersed" model, have been adopted in E–E simulations (Montante and Magelli, 2005). The "for each phase" model resolves the transport equations of k and ε for each of the two phases. In the "mixture" model, the same values for k and ε and the physical properties of the mixture of the two phases are utilized during the resolution of the corresponding equations. Montante and Magelli (2005) compared these models and found that no apparent difference existed between the results of the "for each phase" and "mixture" models. Thus, the "mixture" model has been widely utilized (Khopkar *et al.*, 2006; Kasat *et al.*, 2008; Tamburini *et al.*, 2009). The "dispersed" model solves the k and ε equations only for the continuous phase, and the effect of the discrete phase on the continuous phase and predictions of the turbulence quantities for the discrete phase are included with source terms (Wang *et al.*, 2004a; Murthy *et al.*, 2007; Feng *et al.*, 2012).

It is known that the k–ε models cannot adequately estimate flows with anisotropic characteristics because of the isotropic assumption of turbulence in these models. Feng *et al.* (2012) developed a two-phase explicit algebraic stress model (EASM) to simulate the turbulent solid–liquid flow in a standard stirred tank. Improved results were obtained compared to the k–ε model, but quantitative prediction of the turbulence components such as velocity fluctuations and turbulent kinetic energy was not possible with the EASM.

1.2 Large eddy simulation

Treatment of the continuous phase by using LES has been addressed in very few studies. Derksen (2003) simulated the turbulent flow in a lab-scale stirred tank by using the LES method with the Smagorinsky subgrid scale (SGS) model. In the case of one-way coupling, the continuous flow is not impacted by the presence of particles, i.e., the particles do not perturb the flow field. Thus, the strategies for simulating the continuous phase are the same as those used for single-phase flow. In the two-way coupling simulation, the drag force that the fluid exerts on the particles is fed back to the fluid by a linear interpolation. The simulated results show that the effect of two-way coupling on the averaged flow field is significant but not large. For cases in which the particles carry sufficient momentum to set the surrounding fluid in motion (Derksen *et al.*, 2008), it is necessary to use the two-way coupling simulation for the continuous phase.

An E–L approach with LES for the continuous phase can be adopted for processes that span many integral time scales by using previously stored flow time series (Derksen, 2006). The results obtained using this approach highlighted the importance of SGS motions and models given that the steady-state particle concentration profiles were sensitive to the SGS fluctuation levels. Thus, further discussion of this topic is required.

Ayranci *et al.* (2013) simulated the start-up and subsequent steady-state of a solids suspension process in a baffled tank under strongly turbulent conditions. The solids used were bidispersed particles (glass and bronze) and the solid volume fraction was 1%, making the system a dilute system. The global start-up behavior of the suspension process simulated by the E–L approach with LES was in good agreement with the empirical observations.

The role of stochastic modeling for particle tracking is, in general, much less pertinent in the LES simulation than in RANS-based simulations. The velocity fluctuations in RANS simulations are usually modeled in statistical terms

(Srinivasa and Jayanti, 2007). In LES simulations, provided that certain criteria are met, the motion of particles will be determined primarily by the resolved flow field, and the SGS modeling will have little influence on the particle motion (Derksen, 2003). Therefore, the LES flow field provides more realistic information for fluid and particles than the RANS-based flow field.

1.3 Direct numerical simulation

Studies modeling the continuous phase in solid–liquid suspensions of stirred tanks using DNS are very rare. Sbrizzai *et al.* (2006) investigated the turbulent dispersion of inertial particles in a stirred tank equipped with a Rushton impeller. A second-order finite difference scheme in a cylindrical reference frame was used to directly resolve the flow scale down to the Kolmogorov scale. The effect of the particles on the flow was neglected, thus following the one-way coupling momentum transfer between the two phases. An intermittent Ekman pumping vortex, which is associated with particle resuspension dynamics, was predicted in the unbaffled tank agitated by an eight blade paddle impeller by this approach, and the dimensionless frequency of this vortex was 0.162 (Lavezzo *et al.*, 2009).

Derksen (2012) simulated the solid–liquid flow in a small stirred tank by using DNS based on the Lattice–Boltzmann method. The simulations fully resolved both the turbulent flow and the spherical suspended particles in the tank; the solids volume fraction was about 8%. The smallest turbulent length scale in the stirred tank was estimated to be about half of the grid spacing, which satisfies the typical criterion for sufficiently resolved DNS of turbulence.

In comparison with RANS and LES, DNS resolves turbulent flow fields with a wider range of scales (from the macroscopic scale to the Kolmogorov scale) without modeling and assumptions. Thus, detailed information about the flow field can be provided to describe the motions of suspended particles. Moreover, DNS is an important tool for validating various turbulence models as well as discrete phase models.

2. Models for Discrete Phase

The E–E approach for simulating solid–liquid suspensions considers the particulate phase to be a continuous phase that interpenetrates and interacts with the continuous fluid phase. Therefore, the modeling techniques are almost the same as those described in Section 1.1.

Based on the resolved scale of the discrete phase, point-particle and resolved-particle methods have been used for the E–L approach to simulate the solid–liquid suspension in stirred tanks.

2.1 Point-particle method

In the point-particle method, the finite volume of the discrete phase (particles) is not considered and the flow around the particles is not resolved. The motion of particles is governed by Newton's second law, and their path is tracked in a Lagrangian way. Forces acting on the particles include drag and lift forces from the fluid, body force, and the interparticle force, etc., and various semi-empirical correlations are required to represent these forces. If the continuous phase is simulated by a RANS-based model, a stochastic tracking method is usually required to consider the influence of instantaneous turbulent velocity fluctuations on the particle trajectories (Srinivasa and Jayanti, 2007). For the flow field simulated by LES with high spatial and temporal resolution, the effect of the SGS velocities on the particle behavior is usually insignificant (Derksen, 2003). The SGS part of the drag force was included in the simulations by Derksen (2003) whereas other SGS components were omitted for simplification.

Due to the complexity of particle–particle interaction, its influence is often neglected by invoking certain assumptions (Sbrizzai *et al.*, 2006; Srinivasa and Jayanti, 2007; Lavezzo *et al.*, 2009). Sommerfeld and Decker (2004) found strong nonphysical accumulation of particles near the bottom wall of the tank if the interparticle collisions were not considered. The importance of particle–particle collisions was emphasized by Derksen (2003). In their simulations, all the collisions (particle–wall, particle–impeller, and particle–particle collisions) were assumed to be fully elastic and frictionless. Another assumption of their collision algorithm is that one particle can only collide once with another particle during one time step. The collision algorithm was numerically tested and successfully applied to predict the solids suspension in a stirred tank, and unrealistic build-up of particles close to the bottom wall was avoided.

The point-particle method is usually limited to dilute solid–liquid systems. In dense solid–liquid systems, the finite volume occupied by the particles becomes important relative to the volume of the continuous phase, which is not well represented by the point-particle method. Another reason for this limitation is that the point-particle method generally utilizes single-particle correlations for the hydrodynamic forces acting on the particles.

2.2 Resolved-particle method

Resolved-particle methods take into account the volume and the surface boundary of the suspended particles and the interaction between the flow and the particles. The ultimate function of this method is to achieve completely resolved DNS; that is, all the scales of the surrounding turbulence and the flow scales induced by the particles are fully resolved (Balachandar and Eaton, 2010).

Derksen (2012) investigated the solids suspension process in a stirred tank by utilizing this method. The flow field could be highly resolved by using the Lattice–Boltzmann method, and the typical criterion required by the DNS of turbulence was satisfied. Resolved hydrodynamic forces, unresolved lubrication forces, net gravity, and collisions were included in the linear and rotational motion equations of each individual particle. An immersed boundary method was used to deal with the no-slip boundary conditions at the particle surface. The particle–particle interactions were simulated by using a hard-sphere collision algorithm with restitution and friction coefficients. The restitution coefficient was set to 1.0, and the friction coefficient, which allows particles to transfer linear momentum into angular momentum and vice versa, was set to 0.1.

Figure 1 shows the effect of the Shields number on the instantaneous suspension process after reaching steady-state. The solids are partially suspended when the Shields number is low, whereas they are almost uniformly distributed around the tank when the Shields number is high. The average suspension conditions were also quantitatively analyzed. Although the simulations were performed for a miniature stirred reactor because of computational resources and parallelization, the underlying mechanisms are to some extent universal and relevant for larger-scale stirred reactors.

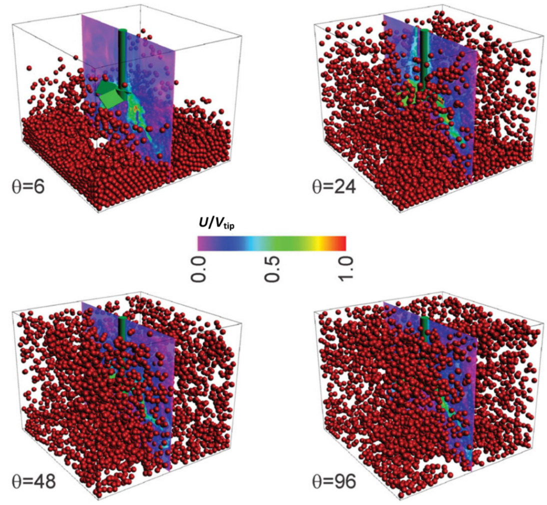

Fig. 1 Influence of Shields number, which is defined as the ratio of the hydrodynamic stress suspending the particles to gravity pulling them to the bottom of the tank, on the instantaneous suspension process after reaching steady-state (Derksen, 2012)

3. Applications of E–E and E–L Models

3.1 Velocity and turbulence components

CFD models can provide detailed information about the flow of a solid–liquid suspension in a stirred tank, but the predictions should be extensively validated before being applied for scale-up or optimization. Guha *et al.* (2008) compared the solids velocities and turbulent kinetic energy predicted by the E–L and E–E models with those measured by using the computer automated radioactive particle tracking (CARPT) technique. LES and the standard k–ε model with mixture properties were respectively used in the E–L and E–E models. The maximum solid hold-up was about 1% (v/v) (2.5% w/w), and the Reynolds number was 74000. Quantitative predictions of the averaged velocity components at different locations were improved when the E–L model was used relative to the results achieved with the E–E model, which is encouraging for extending the application of the former model for stirred tanks.

Derksen (2009) simulated the solid particle mobility in a mixing tank with a Bingham liquid. The drag, gravity, and particle–wall and particle–particle collisions were considered in describing the motions of the particles, and the one-way coupling assumption was reasonable for the cases investigated. The averaged velocity field of the solids was almost identical to that of the liquid, i.e., the slip velocity between the solid particles and the liquid was very small.

In order to verify various CFD models and acquire deeper understanding of the characteristics of solid–liquid suspensions in stirred tanks, systematic experimental data at different solids concentrations must be provided. Montante *et al.* (2012) investigated the effect of the discrete phase on the mean velocity and turbulence levels of the continuous phase and the local solid–liquid slip velocity based on particle image velocimetry measurements. The maximum solids concentration was 0.2% (v/v) due to optical attenuation of the laser sheet across the measurement plane. Guha *et al.* (2007) measured the solid flow dynamics in a solid–liquid stirred tank with a wide range of solids concentrations (2.5–19%) by using the CARPT technique. The ultrasound velocity profiler (UVP) technique was used to measure the local velocities of the solid and liquid phases; the solids loadings ranged from 1 to 7% (v/v) (Sardeshpande *et al.*, 2011). Further experiments considering different geometrical parameters and operating conditions still need to be addressed.

3.2 Solids concentration

The solids concentration distributions have been discussed in most of the published numerical studies because this parameter serves the dual function of providing a qualitative and quantitative description of the suspension quality as well as providing verification of the numerical models and approaches adopted.

Micale *et al.* (2000) compared a simple settling velocity model (SVM) with a two-fluid model and found that both models provided results that were in acceptable agreement with the experimental data for one-dimensional axial concentration profiles. The SVM does not account for the effect of the particle volume fraction and is thus limited to dilute suspension cases.

Various solid–liquid suspension systems with solids fractions ranging from dilute to dense have been simulated by using the E–E approach, and the solid particle distributions have been validated and verified by many researchers (Altway *et al.*, 2001; Barrue *et al.*, 2001; Montante *et al.*, 2001; Špidla *et al.*, 2005; Fletcher and Brown, 2009; Liu and Barigou, 2013; Tamburini *et al.*, 2013). The effects of other parameters including the particle size (Sha *et al.*, 2001; Ochieng and Lewis, 2006b), mixed particles with different densities (Montante and Magelli, 2007), the Schmidt number, the laminar viscosity coefficient (Montante *et al.*, 2002; Shan *et al.*, 2008), and scale-up criteria (Montante *et al.*, 2008) on the solids concentration distribution have also been discussed. A common concern regarding such simulations is the selection of the interphase model due to turbulent flow, which has a significant effect on the predicted results.

The preferential concentration of particles in different regions of a stirred tank was studied by evaluating the deviation from Poisson distribution (Sbrizzai *et al.*, 2006). The distribution of large particles deviated from the randomly distributed state, indicating that their relaxation time was close to the relevant timescale of the flow field.

3.3 Just-suspended speed

Complete suspension of solid particles in the liquid phase is important for ensuring maximum surface area between the two phases, and further energy input for achieving a homogeneous suspension may not be desirable. Thus, the just-suspended speed (N_{js}) becomes an important design parameter. Zwietering (1958) defined the complete suspension state as the state in which all the solid particles are in motion and no particle rests on the bottom of the vessel for more than 1 to 2 s; the corresponding minimum impeller speed is the just-suspended speed. This observation criterion, which is commonly used in experiments, is difficult to apply in the E–E approach; thus, several CFD based methods for determining the N_{js} have been proposed.

Kee and Tan (2002) monitored the simulated instantaneous profiles of the solids volume fraction for the layer of cells adjacent to the bottom of the vessel. They determined the N_{js} to be the impeller speed at which all of the profiles at different locations exhibit steady-state behavior and all of the steady-state values are ∼50% of the initial packed volume fraction.

Wang *et al.* (2004b) recommended examining the simulated axial velocity of the solid phase in the cells closest to the tank bottom at different impeller speeds. If the sign of the velocity is positive for the position where the solid particles are most difficult to be suspended, the corresponding impeller speed can be considered as N_{js}. The limitation of this method lies in the fact that this position must be determined in advance and may change for different impellers. For a baffled tank agitated by a standard Rushton turbine, the center of the bottom of the tank is the above-mentioned critical position.

Murthy *et al.* (2007) predicted the N_{js} by using the standard deviation of solids concentration in a vertical plane and considered the critical value for the normalized standard deviation as 0.75. This value is valid for different impeller designs and is applicable over a wide range of particle sizes and solids loadings. Panneerselvam *et al.* (2008, 2009) combined the standard deviation method and cloud height criteria (i.e., the cloud height is equal to 0.9 times the liquid height) and found the latter to be determinant.

Hosseini *et al.* (2010) calculated the N_{js} via a CFD model by using the tangent intersection method. The average solids concentration in a horizontal plane located 1 mm above the bottom of the tank was calculated, and the relationship of this parameter to the impeller speed was determined. Two tangents to the curve were drawn at the points having the maximum and minimum slopes, and the N_{js} was determined as the intersection of the two tangents (see **Figure 2**).

Based on assessment of the different methods used for determining the N_{js}, Tamburini *et al.* (2012) reported that large differences exist among the different criteria. Their comparison was based on the CFD simulation in a stirred tank equipped with the radially pumping Rushton turbine. The authors suggested a new sufficient suspension concept, which omits a small amount of unsuspended particles (about 2%), to decrease the required power consumption. This concept may be useful in some applications, but it should be carefully considered for processes in which the last small residual fraction of particles is still crucial, such as crystallization. Impeller type and other geometrical parameters exert a significant influence on the criteria in determining the just-suspended speed in CFD models; further studies are thus required.

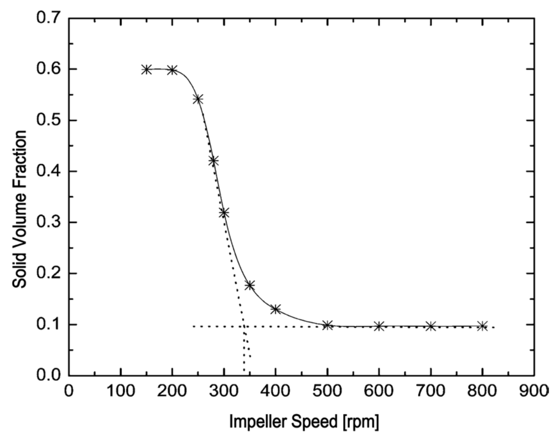

Fig. 2 Use of tangent intersection method to calculate just-suspended impeller speed (Hosseini *et al.*, 2010)

In the E–L approach, Srinivasa and Jayanti (2007) presented a criterion for determining the critical suspension of particles that was similar to the rule used in experiments. They monitored the particle trajectories and normal distances from the lowest point on particle surfaces to the bottom of the vessel for a certain time period. The critically suspended status is determined when the particle does not spend more than 1–5 s on the bottom of the vessel.

3.4 Cloud height

For solids loadings greater than 10 weight percent in a stirred tank, a clear solid–liquid interface usually exists in the upper part of the vessel, and the height of this interface is known as the cloud height (Bittorf and Kresta, 2003). The formation of a clear liquid layer is caused by the axial velocity of the continuous phase being lower than the particle settling velocity (Bittorf and Kresta, 2003; Micale *et al.*, 2004).

Micale *et al.* (2004) compared the empirically determined cloud height with that derived from E–E simulations. The simulated results qualitatively reproduced the main features of the experimental phenomena such as the effect of the solids concentration on the cloud height distribution. Quantitative comparisons showed that more complex interphase models, including particle drag correlations and particle–particle interactions, should be considered to improve the accuracy of the simulated results.

Ochieng and Lewis (2006a) evaluated the cloud height in a fully baffled tank with an elliptical bottom that was agitated by a hydrofoil impeller. In the CFD simulation, the cloud height was determined from the axial profile of the solid volume fraction. The predicted cloud heights were in very good agreement with the experimental results for up to 10% solids loading, whereas the discrepancies increased with increasing solids loading.

Sardeshpande *et al.* (2010) experimentally measured the hysteresis in cloud height, which varies non-monotonically with impeller speed (especially at higher solids loading). The maximum solids loading in their experiments was 7% (v/v). The hysteresis phenomena can be well captured by the CFD models with appropriate initial guess and drag correlations.

3.5 Optimization of geometrical parameters

Hosseini *et al.* (2010) compared the performance of three axial flow impellers, namely Lightnin A100, A200, and A310, at constant power input by using an E–E approach and a standard k–ε model. The A100 impeller was determined to be the most efficient for solid–liquid mixing, whereas the A200 impeller was the least effective for achieving a high degree of homogeneity.

The effect of a draft tube on the solid distribution and mixing time in a stirred tank with a Rushton turbine was discussed by Wang *et al.* (2010) using the E–E approach and an RNG k–ε model. Less homogeneous solids distribution was achieved in the tank with the draft tube relative to the tank without the draft tube, and the mixing time of the former tank was longer than that of the latter. These results may be based on the specific configuration of the draft tube used.

3.6 Particle shape and type

Suspensions of nonspherical particles in stirred tanks are commonly used in process industries, though few corresponding CFD simulations have been reported. Scully and Frawley (2011) investigated the effect of the particle shape on the suspension of prismatic and needle-like crystals by using the E–E approach and the RNG k–ε model. A modified drag force was used to simplify such complex phenomena, and other forces such as the lift force were treated as negligible. The suspension characteristics could be adequately predicted for a range of impeller rotational speeds by applying the custom drag law for non-spherical particles.

Fan *et al.* (2005) simulated the suspension of slender particles in a stirred tank with a Rushton turbine by using the E–E approach and a standard k–ε model. The drag coefficient measured from their experiments with slender particles was utilized to calculate the drag force between the fluid and particles, and the orientations of the slender particles were calculated from the evolution equations of rigid particles. The results showed that the flow field of slender particles was similar to that of equivalent spherical particles, which might be derived from the very low volumetric concentration of 0.02%.

The drawdown of floating particles in stirred tanks was recently investigated by using the E–L approach (Waghmare *et al.*, 2011) as well as the E–E approach (Chen *et al.*, 2012). Khazam and Kresta (2008, 2009) identified the mechanisms of solids drawdown in stirred tanks, including the formation of a stable central vortex, turbulent fluctuations, and mean drag. At present, it is difficult to quantitatively predict drawdown phenomena, especially for cases in which the particles agglomerate and/or trap air and/or have poor wettability.

4. Perspective for E–E and E–L Approaches

Currently, all published E–E simulations dealing with solid–liquid suspensions in stirred tanks handle turbulence by using RANS-based models. This approach is the most suitable for simulating solid–liquid suspensions of engineering relevance because of its lower computational effort and the capability to deal with high solids loading. However, the E–E approach with RANS-based models largely depends upon the quality of the modeling (such as interphase models). Tamburini *et al.* (2011) found that good results could only be obtained by paying special attention to the specification of the interphase drag term. In particular, the influence of free-stream turbulence on the particle drag must be specified to achieve agreement between simulated and experimental data. Khopkar *et al.* (2006) also proposed that assuming the discrete phase to be a continuum requires somewhat more sophisticated modeling of the interphase momentum exchange terms. Thus, the results of these simulations cannot be interpreted in an unambiguous way (Srinivasa and Jayanti, 2007). A shift from RANS-based models to LES or DNS for simulation the turbulence might be promising for the E–E approach.

DNS or LES represent better choices than RANS for simulating the continuous phase using the E–L approach with a point-particle method given that the role of stochastic modeling in particle tracking is much more significant in RANS than in LES; in principle DNS does not require stochastic modeling. This approach is most suitable for dilute polydisperse suspensions, although there are some challenges including the coupling of the particles back to the fluid, particle–particle interaction, and the requirement for extensive computational resources.

The E–L approach employing the resolved-particle method can be considered as a research tool for obtaining a better mechanistic understanding of various suspension phenomena such as the critical condition for suspending particles from the bottom of the reactor, trajectories of just-suspended particles, and particle–particle interactions. Derksen (2012) projected that their highly resolved simulation with resolved particles could be extended to handle lab-scale stirred tanks if a massively parallel computing system is utilized. Such simulations and corresponding experiments should enable investigation of the hydrodynamics as well as the mechanisms of solid–liquid suspensions in lab-scale stirred tanks, and may facilitate improvement of RANS-based models and interphase models used in the E–E and E–L simulations.

Conclusion

A review of the models for simulating solid–liquid suspensions in stirred tanks was presented with focus on the approaches for modeling the effect of the discrete phase on the continuous phase. Various applications of these models were summarized, revealing the wealth of two-phase numerical simulations. The Eulerian–Eulerian approach is suitable for problems of engineering relevance, but reliable models such as interphase models should be provided and a shift from RANS-based models to LES or DNS for simulation of turbulence might be promising. The Eulerian–Lagrangian approach with resolved particles is a prospectively powerful research tool for addressing the underlying mechanisms in solids suspension systems, although certain challenges, including the requirement for massively parallel computing, remain unaddressed.

Acknowledgement

The financial support from the National Natural Science Foundation of China (Nos. 21121064 and 21376016) is gratefully acknowledged.

Literature Cited

Altway, A., H. Setyawan, Margono and S. Winardi; "Effect of Particle Size on Simulation of Three-Dimensional Solid Dispersion in Stirred Tank," *Chem. Eng. Res. Des.*, **79**, 1011–1016 (2001)

Ayranci, I., S. M. Kresta and J. J. Derksen; "Experiments and Simulations on Bidisperse Solids Suspension in a Mixing Tank," *Chem. Eng. Technol.*, **36**, 1957–1967 (2013)

Balachandar, S. and J. K. Eaton; "Turbulent Dispersed Multiphase Flow," *Annu. Rev. Fluid Mech.*, **42**, 111–133 (2010)

Barrue, H., J. Bertrand, B. Cristol and C. Xuereb; "Eulerian Simulation of Dense Solid–liquid Suspension in Multi-Stage Stirred Vessel," *J. Chem. Eng. Japan*, **34**, 585–594 (2001)

Bittorf, K. J. and S. M. Kresta; "Prediction of Cloud Height for Solid Suspensions in Stirred Tanks," *Chem. Eng. Res. Des.*, **81**, 568–577 (2003)

Brucato, A., F. Grisafi and G. Montante; "Particle Drag Coefficients in Turbulent Fluids," *Chem. Eng. Sci.*, **53**, 3295–3314 (1998)

Chen, T., L. Wang, D. Wu, Y. Sun, B. Wu and Z. Li; "Investigation of the Mechanism of Low-Density Particle and Liquid Mixing Process in a Stirred Vessel," *Can. J. Chem. Eng.*, **90**, 925–935 (2012)

Clift, R., J. R. Grace and M. E. Weber; Bubbles, Drops, and Particles, Academic Press, New York, U.S.A. (1978)

Derksen, J. J.; "Numerical Simulation of Solids Suspension in a Stirred Tank," *AIChE J.*, **49**, 2700–2714 (2003)

Derksen, J. J.; "Long-Time Solids Suspension Simulations by Means of a Large-Eddy Approach," *Chem. Eng. Res. Des.*, **84**, 38–46 (2006)

Derksen, J. J., H. E. A. van den Akker and S. Sundaresan; "Two-Way Coupled Large-Eddy Simulations of the Gas–Solid Flow in Cyclone Separators," *AIChE J.*, **54**, 872–885 (2008)

Derksen, J. J.; "Solid Particle Mobility in Agitated Bingham Liquids," *Ind. Eng. Chem. Res.*, **48**, 2266–2274 (2009)

Derksen, J. J.; "Highly Resolved Simulations of Solids Suspension in a Small Mixing Tank," *AIChE J.*, **58**, 3266–3278 (2012)

Fan, L., Z. Mao and Y. Wang; "Numerical Simulation of Turbulent Solid–Liquid Two-Phase Flow and Orientation of Slender Particles in a Stirred Tank," *Chem. Eng. Sci.*, **60**, 7045–7056 (2005)

Feng, X., X. Li, J. Cheng, C. Yang and Z. Mao; "Numerical Simulation of Solid–Liquid Turbulent Flow in a Stirred Tank with a Two-Phase Explicit Algebraic Stress Model," *Chem. Eng. Sci.*, **82**, 272–284 (2012)

Fletcher, D. F. and G. J. Brown; "Numerical Simulation of Solid Suspension via Mechanical Agitation: Effect of the Modeling Approach, Turbulence Model and Hindered Settling Drag Law," *Int. J. Comput. Fluid Dyn.*, **23**, 173–187 (2009)

Guha, D., P. A. Ramachandran and M. P. Dudukovic; "Flow Field of Suspended Solids in a Stirred Tank Reactor by Lagrangian Tracking," *Chem. Eng. Sci.*, **62**, 6143–6154 (2007)

Guha, D., P. A. Ramachandran, M. P. Dudukovic and J. J. Derksen; "Evaluation of Large Eddy Simulation and Euler–Euler CFD Models for Solids Flow Dynamics in a Stirred Tank Reactor," *AIChE J.*, **54**, 766–778 (2008)

Gosman, A. D., C. Lekakou, S. Politis, R. I. Issa and M. K. Looney; "Multidimensional Modeling of Turbulent Two-Phase Flows in Stirred Vessels," *AIChE J.*, **38**, 1946–1956 (1992)

Hosseini, S., D. Patel, F. Ein-Mozaffari and M. Mehrvar; "Study of Solid–Liquid Mixing in Agitated Tanks through Computational Fluid Dynamics Modeling," *Ind. Eng. Chem. Res.*, **49**, 4426–4435 (2010)

Joshi, J. B., N. K. Nere, C. V. Rane, B. N. Murthy, C. S. Mathpati, A. W. Patwardhan and V. V. Ranade; "CFD Simulation of Stirred Tanks: Comparison of Turbulence Models. Part I: Radial Flow Impellers," *Can. J. Chem. Eng.*, **89**, 23–82 (2011a)

Joshi, J. B., N. K. Nere, C. V. Rane, B. N. Murthy, C. S. Mathpati, A. W. Patwardhan and V. V. Ranade; "CFD Simulation of Stirred Tanks: Comparison of Turbulence Models. Part II: Axial Flow Impellers, Multiple Impellers and Multiphase Dispersions," *Can. J. Chem. Eng.*, **89**, 754–816 (2011b)

Kaminoyama, M.; "Review of Visualization of Flow and Dispersion States of Slurry System Fluids in Stirred Vessels," *J. Chem. Eng. Japan*, **47**, 109–114 (2014)

Kasat, G. R. and A. B. Pandit; "Review on Mixing Characteristics in Solid–Liquid and Solid–Liquid–Gas Reactors Vessels," *Can. J. Chem. Eng.*, **83**, 618–643 (2005)

Kasat, G. R., A. R. Khopkar, V. V. Ranade and A. B. Pandit; "CFD Simulation of Liquid-Phase Mixing in Solid–Liquid Stirred Reactor," *Chem. Eng. Sci.*, **63**, 3877–3885 (2008)

Kee, N. C. S. and R. B. H. Tan; "CFD Simulation of Solids Suspension in Mixing Vessels," *Can. J. Chem. Eng.*, **80**, 1–6 (2002)

Khazam, O. and S. M. Kresta; "Mechanisms of Solids Drawdown in Stirred Tanks," *Can. J. Chem. Eng.*, **86**, 622–634 (2008)

Khazam, O. and S. M. Kresta; "A Novel Geometry for Solids Drawdown in Stirred Tanks," *Chem. Eng. Res. Des.*, **87**, 280–290 (2009)

Khopkar, A. R., G. R. Kasat, A. B. Pandit and V. V. Ranade; "Computational Fluid Dynamics Simulation of the Solid Suspension in a Stirred Slurry Reactor," *Ind. Eng. Chem. Res.*, **45**, 4416–4428 (2006)

Lavezzo, V., R. Verzicco and A. Soldati; "Ekman Pumping and Intermittent Particle Resuspension in a Stirred Tank Reactor," *Chem. Eng. Res. Des.*, **87**, 557–564 (2009)

Liu, L. and M. Barigou; "Numerical Modeling of Velocity Field and Phase Distribution in Dense Monodisperse Solid–Liquid Suspensions under Different Regimes of Agitation: CFD and PEPT Experiments," *Chem. Eng. Sci.*, **101**, 837–850 (2013)

Ljungqvist, M. and A. Rasmuson; "Numerical Simulation of the Two-Phase Flow in an Axially Stirred Vessel," *Chem. Eng. Res. Des.*, **79**, 533–546 (2001)

Magelli, F., D. Fajner, M. Nocentini and G. Pasquali; "Solid Distribution in Vessels Stirred with Multiple Impellers," *Chem. Eng. Sci.*, **45**, 615–625 (1990)

Micale, G., G. Montante, F. Grisafi, A. Brucato and J. Godfrey; "CFD

Simulation of Particle Distribution in Stirred Vessels," *Chem. Eng. Res. Des.*, **78**, 435–444 (2000)

Micale, G., F. Grisafi, L. Rizzuti and A. Brucato; "CFD Simulation of Particle Suspension Height in Stirred Vessels," *Chem. Eng. Res. Des.*, **82**, 1204–1213 (2004)

Montante, G., G. Micale, F. Magelli and A. Brucato; "Experiments and CFD Predictions of Solid Particle Distribution in a Vessel Agitated with Four Pitched Blade Turbines," *Chem. Eng. Res. Des.*, **79**, 1005–1010 (2001)

Montante, G., D. Pinelli and F. Magelli; "Diagnosis of Solid Distribution in Vessels Stirred with Multiple PBTs and Comparison of Two Modeling Approaches," *Can. J. Chem. Eng.*, **80**, 1–9 (2002)

Montante, G. and F. Magelli; "Modeling of Solids Distribution in Stirred Tanks: Analysis of Simulation Strategies and Comparison with Experimental Data," *Int. J. Comput. Fluid Dyn.*, **19**, 253–262 (2005)

Montante, G. and F. Magelli; "Mixed Solids Distribution in Stirred Vessels: Experiments and Computational Fluid Dynamics Simulations," *Ind. Eng. Chem. Res.*, **46**, 2885–2891 (2007)

Montante, G., J. R. Bourne and F. Magelli; "Scale-Up of Solids Distribution in Slurry, Stirred Vessels Based on Turbulence Intermittency," *Ind. Eng. Chem. Res.*, **47**, 3438–3443 (2008)

Montante, G., A. Paglianti and F. Magelli; "Analysis of Dilute Solid–Liquid Suspensions in Turbulent Stirred Tanks," *Chem. Eng. Res. Des.*, **90**, 1448–1456 (2012)

Murthy, B. N., R. S. Ghadge and J. B. Joshi; "CFD Simulations of Gas–Liquid–Solid Stirred Reactor: Prediction of Critical Impeller Speed for Solid Suspension," *Chem. Eng. Sci.*, **62**, 7184–7195 (2007)

Ochieng, A. and A. E. Lewis; "CFD Simulation of Solids Off-Bottom Suspension and Cloud Height," *Hydrometallurgy*, **82**, 1–12 (2006a)

Ochieng, A. and A. E. Lewis; "Nickel Solids Concentration Distribution in a Stirred Tank," *Miner. Eng.*, **19**, 180–189 (2006b)

Ochieng, A. and M. S. Onyango; "Drag Models, Solids Concentration and Velocity Distribution in a Stirred Tank," *Powder Technol.*, **181**, 1–8 (2008)

Ochieng, A. and M. S. Onyango; "CFD Simulation of Solids Suspension in Stirred Tanks: Review," *Hem. Ind.*, **64**, 365–374 (2010)

Panneerselvam, R., S. Savithri and G. D. Surender; "CFD Modeling of Gas–Liquid–Solid Mechanically Agitated Contactor," *Chem. Eng. Res. Des.*, **86**, 1331–1344 (2008)

Panneerselvam, R., S. Savithri and G. D. Surender; "Computational Fluid Dynamics Simulation of Solid Suspension in a Gas–Liquid–Solid Mechanically Agitated Contactor," *Ind. Eng. Chem. Res.*, **48**, 1608–1620 (2009)

Pinelli, D., M. Nocentini and F. Magelli; "Solids Distribution in Stirred Slurry Reactors: Influence of Some Mixer Configurations and Limits to the Applicability of a Simple Model for Predictions," *Chem. Eng. Commun.*, **188**, 91–107 (2001)

Sardeshpande, M. V., V. A. Juvekar and V. V. Ranade; "Hysteresis in Cloud Heights during Solid Suspension in Stirred Tank Reactor: Experiments and CFD Simulations," *AIChE J.*, **56**, 2795–2804 (2010)

Sardeshpande, M. V., V. A. Juvekar and V. V. Ranade; "Solid Suspension in Stirred Tanks: UVP Measurements and CFD Simulations," *Can. J. Chem. Eng.*, **89**, 1112–1121 (2011)

Sardeshpande, M. V. and V. V. Ranade; "Computational Fluid Dynamics Modeling of Solid Suspension in Stirred Tanks," *Curr. Sci.*, **102**, 1539–1551 (2012)

Sbrizzai, F., V. Lavezzo, R. Verzicco, M. Campolo and A. Soldati; "Direct Numerical Simulation of Turbulent Particle Dispersion in an Unbaffled Stirred-Tank Reactor," *Chem. Eng. Sci.*, **61**, 2843–2851 (2006)

Scully, J. and P. Frawley; "Computational Fluid Dynamics Analysis of the Suspension of Nonspherical Particles in a Stirred Tank," *Ind. Eng. Chem. Res.*, **50**, 2331–2342 (2011)

Sha, Z., S. Palosaari, P. Oinas and K. Ogawa; "CFD Simulation of Solid Suspension in a Stirred Tank," *J. Chem. Eng. Japan*, **34**, 621–626 (2001)

Shan, X., G. Yu, C. Yang, Z. Mao and W. Zhang; "Numerical Simulation of Liquid–Solid Flow in an Unbaffled Stirred Tank with a Pitched-Blade Turbine Downflow," *Ind. Eng. Chem. Res.*, **47**, 2926–2940 (2008)

Sommerfeld, M. and S. Decker; "State of the Art and Future Trends in CFD Simulation of Stirred Vessel Hydrodynamics," *Chem. Eng. Technol.*, **27**, 215–224 (2004)

Špidla, M., M. Moštěk, V. Sinevič, M. Jahoda and V. Machoň; "Experimental Assessment and CFD Simulations of Local Solid Concentration Profiles in a Pilot-Scale Stirred Tank," *Chem. Pap.*, **59**, 386–393 (2005)

Srinivasa, T. and S. Jayanti; "An Eulerian/Lagrangian Study of Solid Suspension in Stirred Tanks," *AIChE J.*, **53**, 2461–2469 (2007)

Tamburini, A., A. Cipollina, G. Micale, M. Ciofalo and A. Brucato; "Dense Solid–Liquid Off-Bottom Suspension Dynamics: Simulation and Experiment," *Chem. Eng. Res. Des.*, **87**, 587–597 (2009)

Tamburini, A., A. Cipollina, G. Micale, A. Brucato and M. Ciofalo; "CFD Simulations of Dense Solid–Liquid Suspensions in Baffled Stirred Tanks: Prediction of Suspension Curves," *Chem. Eng. J.*, **178**, 324–341 (2011)

Tamburini, A., A. Cipollina, G. Micale, A. Brucato and M. Ciofalo; "CFD Simulations of Dense Solid–Liquid Suspensions in Baffled Stirred Tanks: Prediction of the Minimum Impeller Speed for Complete Suspension," *Chem. Eng. J.*, **193–194**, 234–255 (2012)

Tamburini, A., A. Cipollina, G. Micale, A. Brucato and M. Ciofalo; "CFD Simulations of Dense Solid–Liquid Suspensions in Baffled Stirred Tanks: Prediction of Solid Particle Distribution," *Chem. Eng. J.*, **223**, 875–890 (2013)

Van den Akker, H. E. A.; "Toward a Truly Multiscale Computational Strategy for Simulating Turbulent Two-Phase Flow Processes," *Ind. Eng. Chem. Res.*, **49**, 10780–10797 (2010)

Wadnerkar, D., R. P. Utikar, M. O. Tade and V. K. Pareek; "CFD Simulation of Solid–Liquid Stirred Tanks," *Adv. Powder Technol.*, **23**, 445–453 (2012)

Waghmare, Y., R. Falk, L. Graham and V. Koganti; "Drawdown of Floating Solids in Stirred Tanks: Scale-Up Study Using CFD Modeling," *Int. J. Pharm.*, **418**, 243–253 (2011)

Wang, F., W. Wang and Z. Mao; "Numerical Study of Solid–Liquid Two-Phase Flow in Stirred Tanks with Rushton Impeller. (I) Formulation and Simulation of Flow Field," *Chin. J. Chem. Eng.*, **12**, 599–609 (2004a)

Wang, F., Z. Mao and X. Shen; "Numerical Study of Solid–Liquid Two-Phase Flow in Stirred Tanks with Rushton Impeller. (II) Prediction of Critical Impeller Speed," *Chin. J. Chem. Eng.*, **12**, 610–614 (2004b)

Wang, L., Y. Zhang, X. Li and Y. Zhang; "Experimental Investigation and CFD Simulation of Liquid–Solid–Solid Dispersion in a Stirred Reactor," *Chem. Eng. Sci.*, **65**, 5559–5572 (2010)

Zwietering, T. N.; "Suspending of Solid Particles in Liquid by Agitators," *Chem. Eng. Sci.*, **8**, 244–253 (1958)