Solid-liquid mixing analysis in stirred vessels

ARTICLE in REVIEWS IN CHEMICAL ENGINEERING · JANUARY 2015
Impact Factor: 2.83

4 AUTHORS:

Baharak Sajjadi
University of Malaya
21 PUBLICATIONS  39 CITATIONS

Raja Shazrin Shah Raja Ehsan Shah
University of Malaya
10 PUBLICATIONS  12 CITATIONS

Abdul Aziz Abdul Raman
University of Malaya
219 PUBLICATIONS  909 CITATIONS

Shaliza Ibrahim
University of Malaya
41 PUBLICATIONS  151 CITATIONS

Available from: Baharak Sajjadi
Retrieved on: 24 July 2015
Raja Shazrin Shah, Raja Ehsan Shah, Baharak Sajjadi, Abdul Aziz Abdul Raman* and Shaliza Ibrahim

**Solid-liquid mixing analysis in stirred vessels**

**Abstract:** This review evaluates computational fluid dynamic applications to analyze solid suspension quality in stirred vessels. Most researchers typically employ either Eulerian-Eulerian or Eulerian-Lagrangian approach to investigate multiphase flow in stirred vessels. With sufficient computational resources, the E-L approach simulates flow structures with higher spatial resolution for dispersed multiphase flows. Common turbulence models such as the two-equation eddy-viscosity models ($k$-$\varepsilon$), Reynolds stress model, direct numerical simulation, and large eddy simulation are described and compared for their respective limitations and advantages. Literature confirms that $k$-$\varepsilon$ is the most widely used turbulence model, but it suffers from some inherent shortcomings due to assumption of isotropy of turbulence and homogeneous mixing. Subsequently, the importance of different forces concerning solid particle flotation is concluded. Studies on dilute systems take into account only drag and turbulence forces while other forces have always been ignored. The simulations of off-bottom solid suspension, solid drawdown, solid cloud height, solid concentration distribution, and particle collision are considered for studies involving solid suspension. Different models and methods applied to investigate the abovementioned phenomena are also discussed in this review.

**Keywords:** computational fluid dynamics (CFD); drag force; solid suspension; stirred vessel.

**Abbreviations**

- **ALE** Arbitrary Lagrangian-Eulerian
- **CARPT** Computer automated radioactive particle tracking
- **CFD** Computational fluid dynamics
- **DNS** Direct numerical simulation
- **E-E** Eulerian-Eulerian
- **E-G** Eulerian-Granular
- **E-L** Eulerian-Lagrangian
- **$k$-$\varepsilon$** Two-equation Eddy-viscosity
- **LES** Large eddy simulation
- **MRF** Multiple reference frames
- **PDF** Probability density function
- **RANS** Reynolds averaged Navier-Stokes
- **RNG** Renormalization group $k$-$\varepsilon$
- **RSM** Reynolds stress model
- **SG** Sliding grid

**1 Introduction**

Turbulently agitated vessels where a solid-liquid suspension is produced account for approximately 80% of all industries and are common in leaching process, crystallization process, catalytic reactions, bio-slurry processes, mineral processing, precipitation, coagulations, dissolution, water treatment, and a variety of other applications (Špidla et al. 2005). Optimum performance, accurate control, and reliable design of these equipment are highly dependent on thorough understanding of several phenomena such as turbulence, local dispersed concentration distribution, fluid flow dynamics, system composition, and different equipment configurations (Leng and Calabrese 2004). At present, computational fluid dynamics (CFD) has emerged as an effective and powerful mean in both applied and fundamental research to predict local fluid dynamics, chemical reactions, and related phenomena such as heat and mass transfer in tanks (Van den Akker 2006). However, hydrodynamic simulation in stirred vessels is very complex due to the interaction between the rotating impeller with multiphase dispersion and highly unsteady field of flow.
Therefore, progress on multiphase flow simulations and selection of appropriate models in stirred vessels are far from being fully understood.

Liquid-particle and particle-particle interactions are dependent on dispersed phase volume fraction and should be considered in CFD simulations. The interaction between phases in multiphase stirred vessels is modeled according to the coupling strength between them.

For dilute particle concentrations ($\alpha_p < 10^{-6}$), particle flow can be neglected but fluid flow should be considered (one-way coupling). For intermediate particle concentrations ($10^{-6} < \alpha_p < 10^{-3}$) and above, the effects of continuous phase on particles may be considered regardless of particle interaction (two-way coupling). For high concentrations ($\alpha_p > 10^{-3}$), the interaction between the particles and the particle action on fluid must be accounted for (four-way coupling) (Elghobashi 1994). Hence, by increasing the particle volume fraction, the interaction between the particles and fluid increases, as shown in Table 1. Generally, in systems containing two solid phases along with a liquid as continuous medium, the solid-solid interaction should be considered in the computational model. The methods of Arastoopour et al. (1982) and Gidaspow et al. (1986) are the most famous approaches for investigating these relationships, where the former is applied to the dilute phase and the latter to the dense bed. It is also worth mentioning that Gidaspow’s method (Gidaspow et al. 1986) was modified by Bell et al. (1997) for simulating a two-dimensional (2D) gas-solid fluidized bed containing two different particle sizes.

Tamburini et al. (2009) investigated the transient behavior of an off-bottom solid-liquid suspension from start-up to steady-state conditions inside a mechanically baffled stirred tank equipped with a standard Rushton turbine using the classical Eulerian-Eulerian (E-E) multifluid model approach. They tested different computational approaches in order to compute the particle-fluid and particle-particle interactions since these terms affect both solid suspension and distribution significantly. An excess particle concentration treatment was therefore adopted to compute particle-particle interaction. Particle fluid interactions were assumed to be limited to drag force exchange. These authors observed satisfactory agreement between the modeled and experimental data, suggesting that their modeling approaches were able to capture the main factors affecting particle distribution in stirred dense systems.

The main focus of this review is on collision-free dispersed phase by considering two-way coupling effects. This work is the third part of a review series where the previous two parts focused on gas-liquid (Sajjadi et al. 2012) and liquid-liquid (Sajjadi et al. 2013) systems. This review provides an insight into different approaches in multiphase flow simulation and investigates two terms of momentum balance in solid-liquid systems in stirred vessels. The first term was momentum and stress transfer from continuous to dispersed phase, which was investigated through different turbulence models. The second term was momentum transferred between dispersed and continuous phase, which depends on the force balance on each particle, and the dispersed phase volume fraction. Based on the force balance, the effects of drag and nondrag forces on particles were investigated. The coupling and interactions were, on the other hand, investigated according to the dispersed phase volume fraction. Results from these models for solid-liquid stirred vessel could be used for analyzing suspension quality, drawdown of floating solids, off-bottom complete solid suspension, cloud height, and solid distribution. There are different review papers on experimental methods and geometrical parameters in stirred vessels (Gogate et al. 2000, Van den Akker 2006, Ochieng et al. 2009, Meyer and Deglon 2011).

2 General approaches

2.1 Black-box

The “black-box” viewpoint was the first approach used to study solid flow dynamics in stirred vessels. However, it was not fully predictive and it required experimental information at all conditions. Algebraic slip mixture model was the other approach that assumed that both solid and liquid phases existed at all points of vessel in the form of interpenetrating continua and move at different velocities (Guha et al. 2008).

2.2 Eulerian-Eulerian

The E-E and Eulerian-Lagrangian (E-L) approaches are frequently found in literature. In the former, both of the continuous and dispersed phases are considered as continuum, which can interpenetrate each other. In this approach, several averaging methods (such as time, volume, or ensemble averaging) are used to formulate governing equations, so the particles are modeled with a certain mass to impose the momentum exchange at the point locations of the particles (Ding et al. 2010). Hence,
Table 1  Continuous and dispersed phase interactions.

<table>
<thead>
<tr>
<th></th>
<th>Particle motion</th>
<th>Coupling</th>
<th>Particle volume fraction</th>
<th>Interaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Increasing particle volume fraction</td>
<td>One-way coupling</td>
<td>Dispersed flow</td>
<td>$\alpha_p &lt; 10^{-4}$</td>
<td>1. Continuous fluid affects particles</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Sparse flow</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Two-way coupling</td>
<td>Dispersed flow</td>
<td>$10^{-4} &lt; \alpha_p &lt; 10^{-3}$</td>
<td>1. Continuous fluid affects particles</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Dilute flow</td>
<td></td>
<td>2. Particle motion affects continuous-fluid motion</td>
</tr>
<tr>
<td></td>
<td>Three-way coupling</td>
<td>Dispersed flow</td>
<td>$10^{-3} &lt; \alpha_p &lt; 10^{-2}$</td>
<td>1. Continuous fluid affects particles</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2. Particle motion affects continuous-fluid motion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3. Particle disturbance of the fluid locally affects another particle’s motion</td>
</tr>
<tr>
<td></td>
<td>Four-way coupling</td>
<td>Dispersed flow</td>
<td>$10^{-2} &lt; \alpha_p &lt; 10^{-1}$</td>
<td>1. Continuous fluid affects particles</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2. Particle motion affects continuous-fluid motion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3. Particle disturbance of the fluid locally affects another particle’s motion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4. Particle collision affects motion of individual particle</td>
</tr>
<tr>
<td></td>
<td>Four-way coupling</td>
<td>Dense flow</td>
<td>Collision-dominated flow</td>
<td>$\alpha_p &gt; 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2. Particle motion affects continuous-fluid motion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3. Particle disturbance of the fluid locally affects another particle’s motion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4. Particle collision affects motion of individual particles</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5. Particles move as a group with high frequency of collisions</td>
</tr>
<tr>
<td></td>
<td>Four-way coupling</td>
<td>Dense flow</td>
<td>Contact-dominated flow</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2. Particle motion affects continuous-fluid motion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>3. Particle disturbance of the fluid locally affects another particle’s motion</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>4. Particle collision affects motion of individual</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>5. Particles have a high frequency of contact</td>
</tr>
</tbody>
</table>
one calculates the average local velocity, volume fraction, and other parameters, not the properties of each individual particle (van Wachem and Almstedt 2003). In the Eulerian approach, most researchers have used monosize particle. Ochieng and Lewis (2006a) used a polydisperse approach to investigate particle size distribution and solid concentration for high-density (nickel) particles and clearly showed that this assumption could not accurately predict experimental results for high-density particles (Ochieng and Lewis 2006a).

2.3 Eulerian-Lagrangian

In the E-L approach, the continuous phase is treated in an Eulerian framework whereas the motion of dispersed phase is simulated by solving the force balance of each particle.

Briefly, since the E-L approach tracks the particles individually, it produces more reflective results and can handle complex phenomena involving particle size, composition, distribution agglomeration, and disaggregation (Farzpourmachiani et al. 2011). However, the E-L approach faces three problems, which are i) false fluctuations of the continuous phase velocity that occur when dispersion passes through the interface of the computational grid and causes sudden changes in the local volume fraction, ii) the amplitude of false velocity fluctuation increases when a small grid is applied, and iii) as the volume fraction of the dispersed phase increases, the interaction between the two phases increases too, which cannot be accounted for by this method due to considerably high demand of computational cost. As a solution for the second problem, Kitagawa et al. (2001) presented a calculation method to convert dispersion to continuous phase interaction, which was accompanied by spherical dispersion migration. They used Gaussian and sine wave filtering function to convert discrete dispersion volume fractions to a spatially differentiable distribution, so that 3D continuous phase flow structures induced by rising spherical bubbles and/or settling solid particles were demonstrated (Kitagawa et al. 2001). For the third problem, it potentially worsens as the calculation requires the time history of the stationary mean of two-phase flow for a long period of time, which increases the computational demand (Ochieng and Onyango 2008, 2010). In view of these problems, 3D flow simulation of this approach is more applicable in dilute systems (Derksen 2003, Yeoh et al. 2005). In the E-E approach, the interaction between the phases is accounted for through source terms and flow field is solved for both phases.

2.4 Arbitrary Lagrangian-Eulerian

It should be noted that in Eulerian description of solids, the expression $X = x + u$ holds and the mathematical models could be derived using either the Eulerian description $(x, t)$ or the Lagrangian description $(\bar{x}, t)$. The two descriptions are similar in terms of displacement, $u$. However, there would be a restriction in fluid at the fixed location, $X$, material transport, and the current position of some material particle, but without knowledge of displacement $u$. Many recent published works switched to arbitrary Lagrangian-Eulerian (ALE) as a starting point for designing various computational strategies for computing liquid-solid interaction evolution. There is no basic dependence on particles, and ALE treats the computational mesh as a reference frame that may be moving with arbitrary velocity, $\bar{V}$. In the choice of $X$, Eulerian and Lagrangian descriptions are derived from a single mathematical model, which is subsequently applied for numerical computations. Since 1981, ALE approaches have been used in a wide range of solid-liquid-based aspects, i.e., fluid-solid interaction, free surface problems, deforming-spatial-domain, stabilized space-time, etc. In most recent works using ALE, Sankaran et al. (2009) developed a coupled and unified solution method for fluid-structure interactions. Another work by Farhat et al. (2010) considered various time integration schemes for fluid-solid interaction problems using this approach. A dual-primal finite element tearing and interconnecting method was considered by Li et al. (2012) in order to solve a class of fluid-solid interaction problems in the frequency domain using the ALE approach. Wang et al. (2011) improved various algorithms for load computation in embedded boundary methods and interface treatment for fluid-structure and fluid interaction problems through the ALE approach. Grétarsson et al. (2011) investigated numerically stable fluid-structure interactions between compressible flow and solid structures. Amsallem and Farhat (2012) considered the stability of linearized reduced-order models with application to fluid-structure interaction. Subsequently, Wang et al. (2012) considered computational algorithms for tracking dynamic fluid-structure interfaces in embedded boundary methods.

In mentioned approaches, there are two basic equations that should be solved: continuity and momentum balance equations, as given in Eqs. (1) and (2), respectively.

$$\frac{\partial}{\partial t} (\alpha_i \rho_i) + \frac{\partial}{\partial x_i} (\alpha_i \rho_i U_i) = \Gamma$$  

and
The Eulerian approach is based on the Eulerian model wherein the solids are considered as a pseudo-fluid. Therefore, the pseudo-fluid physical properties, such as solid stress, pressure, and viscosity, are derived from the kinetic theory of granular flow. Continuity and momentum equations are also solved in this approach. It also includes an additional transport equation for granular temperature. The solid phase momentum equation includes an additional solid pressure term that can be written in the form of

$$\sum_{k=1}^{n} (R_{p} + m_{i} \dot{u}_{i})$$

where the subscript fs accounts for the exchange between the operational phases. The coupling between the phases is obtained through interphase exchange coefficients and pressure term, which are determined from the kinetic theory of granular flow (Ding and Gidaspow 1990). This approach is more accurate for processes containing high particle concentrations.

### 3 Stress tensor from continuous phase

Turbulence treated through the terms of stress tensor ($T_{k}$) in the momentum equation balance is shown in Eq. (4):

$$\bar{T}_{k} = \alpha_{k} (\mu + \mu_{k}) \left( \frac{\partial u_{j}}{\partial x_{i}} + \frac{\partial u_{i}}{\partial x_{j}} \right) - \alpha_{k} \frac{\partial}{\partial x_{i}} (\rho \dot{u}_{j} \dot{u}_{i})$$

(4)

The term $\rho \dot{u}_{j} \dot{u}_{i}$ introduces Reynolds stresses:

$$\rho \dot{u}_{j} \dot{u}_{i} = \frac{2}{3} \rho k \delta_{ij} + (\mu_{k}) \left( \frac{\partial U_{j}}{\partial x_{i}} + \frac{\partial U_{i}}{\partial x_{j}} \right)$$

(5)

Two main categories of turbulence models are available through coupling of this term with the others in the momentum balance equation. The first category under the Lagrangian approach includes direct numerical simulation (DNS), large eddy simulation (LES), and stochastic modeling. The second category includes Reynolds averaged Navier-Stokes (RANS) and probability density function (PDF) modeling, which are collectively called the Eulerian approach.

Since the Lagrangian framework suffers from limitations of high number of dispersed phase, a Eulerian framework is more useful. RANS and PDF are two important models in this regard. The related equations for these models for dispersed phase statistical properties are in the form of “fluid” equations based on the Eulerian framework.

RANS equations are divided into two categories: Reynolds stress model (RSM) and eddy-viscosity model. The two-equation eddy-viscosity models ($k-\varepsilon$) are based on turbulent kinetic energy ($k$) and energy dissipation rate ($\varepsilon$). Standard $k-\varepsilon$, renormalization group $k-\varepsilon$ (RNG), and realizable $k-\varepsilon$ are three different appearances of the $k-\varepsilon$ family’s model; $k-\omega$ is another member of this group, where $\omega$ has been replaced by turbulence frequency ($\omega$).

In the situation of low dispersed phase, the RANS method represents a good tradeoff between the accuracy and computational costs (Petitti et al. 2010). However, it suffers from some shortcomings due to assumption of isotropic turbulence and homogeneous and underprediction of energy dissipation rate. Osman and Varley (1999) found that the predicted mixing time was two times higher than the experimental results due to underestimation of mean velocity near the Rushton turbine. Jaworski et al. (2000) showed an overpredicted value of mixing time using standard and RNG $k-\varepsilon$ due to high underprediction of mass exchange between the four distinct axial-radial circulation loops at the boundary between the circulation loops of upper and lower impeller, whereas $k-\omega$ yielded the smallest values of effective diffusivity in the impeller region.

However, $k-\varepsilon$ can accurately predict the length and intensity of the trailing vortices generated off impeller blades in stirred tanks but requires a large number of modeled revolutions to obtain good statistical average (Singh et al. 2011). Guha et al. (2008) carried out a systematic experimental investigation of solid hydrodynamics in dense solid-liquid suspensions by the computer automated radioactive particle tracking (CARPT) technique and CFD simulation. They validated the CFD results of averaged solid velocities, turbulent kinetic energy, and solid sojourn time distribution using the results from CARPT technique. They also investigated the ability of LES along with the Euler-Euler approach in modeling solid-liquid stirred vessels. They reported that LES and the Euler-Euler model could not capture the difference between the top and bottom flow patterns. In spite of the observed mismatch, the simulation results were in reasonably good agreement with the experimental data for mean and standard deviation of solid sojourn times in...
the stirred vessel. PDF modeling is the most recent technique. In this method, the transition between the Lagrangian and Eulerian frames is modeled initially by using the Liouville theorem (Monaghan 2005). The closure problems are then solved to achieve closed PDF equation and the moments of the PDF equation should be taken. These equations are related to baro-diffusion, turbulent thermal diffusion, and turbophoresis. The phase space variables make up various PDF models. The applied closure scheme and the researcher’s ability to predict selected statistical properties of the fluid are the determining factors on accuracy of PDF equation. Generally, the result of PDF method contains more information than that of RANS models.

Some researchers have also used the LES method, which is able to overcome $k$-$\varepsilon$ limitations for investigations of unsteady behavior in turbulent flow. In LES, large-scale eddies are resolved, and the small scales, which are isotropic in nature, are modeled using subgrid-scale models. The major role of subgrid-scale models is to provide proper dissipation for the energy transferred from the large-scale to the small-scale eddies (Joshi et al. 2011). LES is not fine-tuned for quick process design validation and it requires rather long computational time. There has not been any validation for slurries with high solid concentrations using LES, although it is still easier to recognize fluctuations in comparison to RANS (Hartmann et al. 2004).

DNS is another option that resolves all time scales for which the basic equations are constructed without turbulence and interface models. This is done by direct integration of continuity, momentum, and energy equations in high-order numerical schemes on a sufficiently fine grid. Besides, the assumptions involved in Navier-Stokes equation are still arguable especially in two-phase flows. Thus, solving of flow around the particles is not possible in this model. Therefore, physical models should be considered to describe the interactions between the two phases. This argument becomes much stronger when the two-way coupling between the phases is considered. Generally, DNSs of two-phase turbulent flows are categorized in three different groups: isotropic homogeneous, anisotropic homogeneous, and inhomogeneous flows. In isotropic homogeneous flows, the average properties of random motion do not change under reflection or rotation of the coordinate system. Besides, they are independent of position in the fluid. Therefore, only one component is presented for Reynolds stress tensor. In anisotropic homogeneous flow, the turbulence of all components should be considered, whereas in inhomogeneous flow, these values can differ from two different locations in the flow. This method also provides details on fluctuations and particle flow properties.

In contrast to DNS, LES provides more satisfying results at high Reynolds numbers. LES can provide details of flow field that cannot be obtained by RANS, but it cannot offer details on small-scale fluctuations (Derksen and Van den Akker 1999). In other words, LES provides a solution for turbulence with larger scales while smaller scales are presented in the form of statistical average. Therefore, the interaction between different scales of turbulence and particles remains an open question. Since dissipation rate cannot be solved during LES, it is considered posteriori and is strongly dependent on subgrid-scale model used in the simulations (Delafosse et al. 2008). Generally, literature confirms that RANS-based models (especially $k$-$\varepsilon$) are the most widely used turbulence model in spite of its shortcomings because RANS-based models assume the isotropy of turbulence and homogenous mixing, which are suitable particularly for very high Reynolds number in unbaffled stirred reactors. In addition, it is worth mentioning that LES and DNS approaches are also more accurate for turbulent fluid mixing but more computing demanding (Hartmann et al. 2004, Singh et al. 2011). The related equations considering the mentioned turbulence models are in Table 2.

In conclusion, the $k$-$\varepsilon$ turbulence model is the most widely used for solid-liquid systems. Dispersed, per phase, homogeneous, and asymmetric are the main extensions of the standard $k$-$\varepsilon$ turbulence model for two-phase turbulent fluid fields.

In the per phase approach (also named phase-specific), the turbulence equations, along with the additional terms referring to the modeling of interphase transport of $k$ and $\varepsilon$, are considered for each phase.

In the homogeneous formulation, only one $k$ and one $\varepsilon$ equations are considered and the values are shared between the phases while the physical properties of the mixture are adopted. No interphase turbulence transfer terms are employed for the transport equations for $k$ and $\varepsilon$.

The dispersed approach is more suitable for dilute suspensions. In this expression, fluctuating quantities of the particles are solved as functions of the mean properties of the carrier phase and the ratio of eddy-particle interaction time and the particle relaxation time. Carrier phase turbulence is modeled through the standard $k$-$\varepsilon$ model involving extra terms that account for the effect of the particles on the carrier phase (Feng et al. 2012).

The asymmetric $k$-$\varepsilon$ is more applicable for dense solid-liquid suspensions where $N\leq N_{ij}$. In this formulation, many particles may be unsuspended under partial suspension conditions, and therefore, no turbulent viscosity was accounted for the particles and only the turbulence of the continuous phase was calculated (Tamburini et al. 2011).
Table 2 Summary of turbulence models.

<table>
<thead>
<tr>
<th>Model</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>RANS</td>
<td></td>
</tr>
<tr>
<td>Two eddy viscosity models</td>
<td>$\rho \left( C_{1,s} \frac{\varepsilon}{k} C_{2,s} \frac{\varepsilon}{k} \right)$</td>
</tr>
<tr>
<td>Standard $k$-$\varepsilon$ model</td>
<td>$C_{1,s}=0.09, C_{1,s}=1.44, C_{2,s}=1.92, \sigma_{k,s}=1, \sigma_{\varepsilon,s}=1.314$</td>
</tr>
<tr>
<td>RNG $k$-$\varepsilon$ model</td>
<td>$C_{1,s}=0.0845, C_{1,s}=1.42, C_{2,s}=1.68, \sigma_{k,s}=\sigma_{\varepsilon,s}=0.719, \eta=4.8, \beta=0.012,$</td>
</tr>
<tr>
<td>Realizable $k$-$\varepsilon$ model</td>
<td>$C_{1,s}=0.09, C_{1,s}=1.9, \sigma_{k,s}=1, \sigma_{\varepsilon,s}=1.2, \eta=6E_k, E'=2E_kE'_f, E'_f=0.5 \left( \frac{\partial u}{\partial x_j} \frac{\partial u}{\partial x_i} \right)$</td>
</tr>
<tr>
<td>$k$-$\omega$ model</td>
<td>$v_i = \frac{k}{\omega}, \omega = \max \left( \omega, C_{\omega} \frac{2S \overline{S}}{\rho} \right)$</td>
</tr>
<tr>
<td>$\alpha=0.52, \beta=0.5, \beta=0.09, \alpha=0.5, \eta=100 \omega$</td>
<td></td>
</tr>
<tr>
<td>$\sigma'=0.6, \beta_f=1+85 \chi_{\omega}, \chi_{\omega} = \frac{1}{3} \overline{\overline{u'}} \overline{\overline{u'}} \overline{\overline{\omega}}$</td>
<td></td>
</tr>
<tr>
<td>$\sigma_f=0$ for $\overline{\partial k} \overline{\partial \omega} \overline{\partial x_j} \overline{\partial x_i} &lt; 0$</td>
<td></td>
</tr>
<tr>
<td>$\alpha_f=0.125$ for $\overline{\partial k} \overline{\partial \omega} \overline{\partial x_j} \overline{\partial x_i} &gt; 0$</td>
<td></td>
</tr>
<tr>
<td>$\alpha_f=0.82, C_f=0.09$</td>
<td></td>
</tr>
<tr>
<td>LES</td>
<td></td>
</tr>
<tr>
<td>$\frac{\partial u_j}{\partial t} + u_i \frac{\partial u_j}{\partial x_i} = - \frac{\partial}{\partial x_i} \left( u_j \frac{\partial u}{\partial x_j} \right) - \frac{1}{Re} \frac{\partial^2 u_j}{\partial x_i \partial x_j} \overline{u' \overline{u'}}$</td>
<td></td>
</tr>
<tr>
<td>$\tau_{ij}^{ss} = u_i u_j, \tau_{ij}^{ss} = 2 \nu \overline{u' \overline{u'}}$</td>
<td></td>
</tr>
<tr>
<td>$L = \min (kd, C_L V_i^{1/3})$</td>
<td></td>
</tr>
</tbody>
</table>

Comparing the mentioned models, the homogeneous $k$-$\varepsilon$ turbulence model provides satisfactory representation of the particle distribution throughout the system in cases including dense suspensions in stirred vessels (Montante et al. 2001a, Micale et al. 2004, Montante and Magelli 2005, Khopkar et al. 2006, Kasat et al. 2008, Tamburini et al. 2009).

Further details about the turbulence models are discussed in Sajjadi et al. (2012).

4 Dispersed and continuous phase interaction

Another important term in momentum balance equations is the momentum transfer between the particles (dispersed phase) and liquid (continuous phase), as shown by Eq. (6). The value is dependent on the dispersed phase volume fraction ($\alpha$) and the momentum transferred ($F_{IK}$):
\[ \alpha_k = \frac{1}{V_{cell} \Delta t} \sum_{n} \left( \sum_{k} (F_k) \Delta t \right), \]  

where \( V \) is the volume of the cell and \( \Delta t \) is the time step. The last term is the summation of drag and nondrag forces. Additionally, the particle velocities can be calculated using Eq. (7) by solving the force balance on each particle:

\[ m_b \frac{du}{dt} = F_d + F_f + F_p + F_T + F_M. \]  

The \( m_b \) and \( u \), on the left-hand side of Eq. (7) represent particle mass and velocity, respectively. The right-hand section is the summation of all forces acting on the particle that are divided into two major groups including drag and nondrag forces (Buffo et al. 2011).

### 4.1 Nondrag forces

Nondrag forces include turbulent dispersion (\( F_{pD} \)), lift force, (\( F_L \)) and virtual mass (\( F_{MV} \)). Turbulent dispersion force denotes the effect of turbulent fluctuations on effective momentum transfer. In the simulation of solid suspension in stirred vessels, turbulent dispersion force is significant when the particle size is smaller than the turbulence eddies (Wadnerkar et al. 2012). Turbulent dispersion force appears in the momentum equation for Favre averaging approach, but it appears as a function of Schmidt number in the continuity equation for time-averaging approach (Ochieng and Onyango 2010).

The lift force represents traverse force caused by rotational strain and is significant when there is a large velocity gradient or strong vorticity in the continuous phase (Taghavi et al. 2011). In stirred vessels, velocity gradients in vicinity to the impeller are more than those in the bulk region, so the magnitude of lift force is much smaller at the region far away from the impeller.

Virtual mass force denotes an inertial force that is caused by relative acceleration of phases due to movement of particles and is significant only when there is strong acceleration. In other words, when the dispersed phase density is much smaller than the continuous phase density (Khopkar et al. 2006), the mentioned forces are significant in vicinity to the impeller blades and wall lubrication force tends to push dispersed phase away from the wall. Detailed descriptions on nondrag forces and turbulent dispersion force were given by Lahey et al. (1993) and Lopez de Bertodano (1998).

### 4.2 Drag force

Drag force represents interphase momentum transfer due to disturbance. Drag and turbulence forces overcome other forces in stirred vessels due to the mechanical energy of liquid bulk and its turbulence. These forces cause solid particles to draw down, and other forces may be considered depending on the fluid flow properties as well as particle and fluid physical properties (Khazam and Kresta 2008). The relative magnitude of drag and gravitational forces is given by Archimedes number (\( Ar \)). The drag force is more important for smaller particles, which have lower values of \( Ar \), where terminal velocity has less influence on the flow field (Ochieng and Lewis 2006b). Drag models affect CFD simulations for solid-liquid stirred reactors. In these systems, the interphase drag coefficient (\( C_D \)) is a complex function of a drag coefficient in a stagnant liquid (\( C_{D0} \)), prevailing turbulence level, and solid holdup present in the reactor. If the surrounding liquid is turbulent, the prevailing turbulence is expected to influence effective drag coefficient on particles. By assuming standard drag coefficient (quiescent flow), the effect of turbulent eddies on motion of dispersed phase is often ignored. This results in large errors in simulation of dispersed phase concentration profiles for a turbulent flow. It is worth noting that the magnitude of the effect increases with both mean turbulent energy dissipation rate and particle size. Flow field around solid particles is also affected by microscale turbulence instead of inertial-scale turbulence, so interphase drag coefficient is affected by microscales (Tamburini et al. 2011).

Drag coefficient is also influenced by the relative intensity of turbulence in a free stream turbulent flow and is defined as the ratio of the root-mean-square of fluid velocity to mean particle-liquid relative velocity. Brucato et al. (1998) and Mersmann et al. (1998) explained that if the ratio of particle diameter to Kolmogoroff eddy size (\( d_p/\lambda \)) was more than 5, the influence of free stream turbulence on drag force had to be considered; but if the ratio was <5, the interaction between the energy dissipating eddies and particles was negligible. A constant drag coefficient may be used for such particle size because the drag coefficient is not affected by turbulence (Ochieng and Onyango 2008).

Generally, three methods are available to compute drag forces. The first and simplest approach, namely, fixed-\( C_D \), is based on standard drag curve that computes the value for a single particle settling at its terminal velocity in a silent fluid. This approach is more suitable for dilute systems and low-Reynolds-number flows. The second is slip-\( C_D \), which considers \( C_D \) variables in each cell.
Table 3 Drag models.

<table>
<thead>
<tr>
<th>Model</th>
<th>Note</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{D0} = \max \left( \frac{24}{Re} \left(1 + 0.15 \Re_0^{0.44}, 0.44 \right) \right)$, $\Re_0 = \frac{d_U}{\nu}$</td>
<td>– Applicable on spherical and single particle immersed in unidirectional flow</td>
<td>Schiller and Naumann 1935</td>
</tr>
<tr>
<td>$C_D = \frac{C_D}{C_{D0}} \left[ 1 + 8.76 \times 10^{-4} \left( \frac{d_p}{\lambda} \right)^3 \right]$</td>
<td>– Accounts for free stream turbulence through the Kolmogoroff length scale</td>
<td>Montante et al. 2001b</td>
</tr>
<tr>
<td>$C_D = \frac{\alpha_1^{0.5} \max \left( \frac{24}{Re} \left(1 + 0.15 \Re_0^{0.44}, 0.44 \right) \right)}{C_{D0}} \frac{\Re_p}{\alpha_1 \Re_p}$</td>
<td>– Applicable for dilute systems</td>
<td>Wen and Yu 1966</td>
</tr>
<tr>
<td>$C_D = \frac{150 \alpha_1 \rho_s \left[ \frac{7 \alpha_1 \rho_s | \bar{v}_s | \bar{v}_s}{4 d_s} \right]}{(1 - \epsilon_1 \Re_p^{0.644}) \alpha_1}$</td>
<td>– Applicable for immersed single particle</td>
<td>Ergun 1952</td>
</tr>
<tr>
<td>$C_D = \frac{24}{\Re_s}$</td>
<td>– Applicable for unidirectional flow</td>
<td></td>
</tr>
<tr>
<td>$K_w = \frac{3 \alpha_1 \rho_s \left[ \frac{| \bar{v}_s | \bar{v}_s}{d_s} \right]}{\Re_s^{0.644}}$</td>
<td>– Applicable for immersed single particle</td>
<td></td>
</tr>
<tr>
<td>$C_D = \frac{24}{\Re_s}$</td>
<td>– Applicable for unidirectional flow for single particle immersed in a unidirectional flow</td>
<td></td>
</tr>
<tr>
<td>$K_w = \frac{150 \alpha_1 \rho_s \left[ \frac{| \bar{v}_s | \bar{v}_s}{d_s} \right]}{(1 - \epsilon_1 \Re_p^{0.644}) \alpha_1}$</td>
<td>– Provided satisfactory results for suspended solids only</td>
<td></td>
</tr>
<tr>
<td>$K_w = \frac{3 \left(1 + \alpha_1 \Re_p \right)}{2} \frac{\alpha_1 \rho_s \left[ \frac{| \bar{v}_s | \bar{v}_s}{d_s} \right]}{\Re_s^{0.644}}$</td>
<td>– Applicable for solid-solid interaction in liquid-solid-solid systems of the interphase momentum transfer between two dispersed solid phases</td>
<td>Gidaspow 1994</td>
</tr>
<tr>
<td>$C_D = \frac{0.6 + 0.4 \tanh \left( \frac{16 d_s}{\lambda} \right)}{2}$</td>
<td>– Does not account the influence of particle density</td>
<td>Penilli et al. 2001</td>
</tr>
<tr>
<td>$C_D = \frac{1.876 \times 10^{-4} \left( \frac{d_p}{\lambda} \right)^3}{\Re_s^{0.644}}$</td>
<td>– Accounts for free stream turbulence through the Kolmogoroff length scale</td>
<td>Khopkar et al. 2006</td>
</tr>
<tr>
<td>$U \frac{U}{U_i} = 0.6 + 0.32 \tanh \left( \frac{16 \lambda}{d_s} \left( \frac{\rho_s \bar{v}_s}{\rho_i} \right)^{0.5} \right)$</td>
<td>– Gives reasonable prediction in solid-liquid systems</td>
<td>Fajner et al. 2008</td>
</tr>
</tbody>
</table>

In relation to slip velocity. The third approach is turb-$C_D$ (Brucato et al. 1998), which considers the influence of free-stream turbulence upon drag interphase force. Table 3 shows a number of drag models available to estimate drag force in solid-liquid systems. In many CFD simulations, these models are used in RANS equations.
Tamburini et al. (2009) investigated dense solid-liquid off-bottom suspension inside a stirred tank and focused on different computational approaches to compute drag interphase force. They found that a simple modeling of interphase drag was practical and sufficient to correctly predict the suspension height of a solid-liquid suspension. They used three different equations to account for the effects of solid concentration on interphase drag force. The reported turb-$C_D$ simulation results were in better agreement with the experimental result in comparison to the fixed-$C_D$ simulations (Tamburini et al. 2009). In the same work, they also reported that Brucato’s model (Brucato et al. 1998) predicted a much higher drag coefficient for $d_p/\lambda$ ratios (Tamburini et al. 2011). The equations cater for low solid fractions in the upper clear liquid layer, intermediate volume fractions inside the suspension, and high solid concentrations near the tank bottom, respectively.

### 4.2.1 Drag models

A variety of drag models available in the literature are summarized in Table 3. Dependency of drag on volume fraction and density are always taken into consideration (Lane et al. 2005, Fajner et al. 2008), except for low-Reynolds-number and dilute systems, in which particle drag is given by Stokes law. Turbulent fluctuations increase and significantly affect the predictions at high Reynolds number. The drag and turbulence thus become important for stirred tank systems. Besides, the contribution of turbulent dispersion force is significant only when the particle size is smaller than the turbulent eddies. Therefore, in stirred vessels where the largest energy containing eddy (in mm) is 10 times more than the particle size, the role of the turbulent dispersion is entirely prominent (Sardeshpande and Ranade 2012). There should then be a model that takes turbulence into account, since the impact of turbulence on the drag increases with increasing Reynolds number. In view of this, Brucato’s model (Brucato et al. 1998) is more suitable in stirred vessel. This model is based on the ratio of particle diameter and Kolmogorov length scales, which is dependent entirely on turbulence.

Therefore, change in turbulence changes the drag. This model has been successfully employed by some authors (Montante et al. 2001a, Montante and Magelli 2005). However, this model does not capture complete suspension of solid particles in stirred vessels and when there are more than 10% of solid particles. In view of this, the predicted value may deviate from the real value, with overprediction of the height of solid suspension. A mismatch in the radial and tangential components of velocity at impeller plane was also reported by Panneerselvam and Savithri (2008). Some other authors (Ljungqvist and Rasmuson 2001, Montante et al. 2001a) have also reported that this model gives the best results in systems with low particle hold-up. Considering these problems, Khopkar et al. (2006) modified Brucato’s model (Brucato et al. 1998) by decreasing the value of the proportionality constant by about 10 times ($K=8.76\times10^{-5}$) for systems containing particle size $<655$ μm and solid hold-up $<16\%$. Therefore, the model clearly indicates that the effective drag coefficient depends on the ratio of the particle diameter to the Kolmogorov length scale. Khopkar et al. (2006) reported that suspension height was well predicted by the modified correlation, substantiated by the experimental data. The other authors have also indicated this result (Sardeshpande et al. 2010). Hence, the proportionality constant appearing in Brucato’s model (Brucato et al. 1998) needs to be reduced for higher solid loading and larger particle Reynolds numbers (Khopkar et al. 2006). Additionally, this model can be combined with the $k$-$\varepsilon$ model; thus, it is more appropriate for stirred tanks.

Gidaspow’s (1994) model is another widely used model for solid-liquid systems. The model is a combination of Wen-Yu’s (Wen and Yu 1966) model for low solid loading rate ($\phi_s<0.2$) and Ergun’s (1952) model for high solid loading rate ($\phi_s>0.2$). Gidaspow’s (1994) model is more appropriate for systems with relatively higher solid loading rate compared to other models. Ochieng and Lewis (2006b) compared Gidaspow’s (1994) model and Brucato’s model (Brucato et al. 1998) in both dilute and dense systems (1–20%w/w with density of 9800 kg/m$^3$) and reported that both models produced similar results.

Ochieng and Onyango (2008) compared different drag models that account for the effect of free stream turbulence, including those based on Reynolds number only. They also studied those models that account for solid volume fraction for predicting solids suspension in stirred vessels and found that drag models based on solids volume fraction produced comparatively better results.

Ljungqvist and Rasmuson (2001) used two phase flow field in an axially stirred vessel containing nickel particles of 75 μm diameter to investigate slip velocity distribution and compared the performance of four different drag models: Ishii-Zuber model (Ishii and Zuber 1979), Ihme’s model (AEAT 2003), Brucato’s model (Brucato et al. 1998), and Schiller-Naumann’s model (Schiller and Naumann 1935). In their study, $\lambda/d_p$ ratio was high enough so that $C_D$ did not increase relatively to $C_{D_{in}}$; thus, they did not observe any difference in prediction by those models. Besides, they reported that radial and tangential components were
severely underestimated due to overestimation of axial slip. They further estimated slip velocity from the settling velocity of particles in a quiescent liquid (Andersson theory; Andersson 1986). However, slip velocity derived from this method deviated from the measured values. This was because drag in viscous Reynolds number region was increased by free stream turbulence. Besides, enhanced drag also resulted in lower slip velocities and overestimation of the axial slip (Ljungqvist and Rasmuson 2001). In other words, the magnitude of drag increases with turbulence and influences slip velocity between the primary and secondary phases. Hence, underprediction of turbulent kinetic energy eventually results in underprediction of slip velocities. Derksen (2003) reported dominance of high slip velocity in the impeller zone by comparing slip velocities in terms of linear and rotational Reynolds number. The author also pointed out that although all drag models were able to capture high slip velocities in this region, only modified Brucato’s drag model (Brucato et al. 1998) yielded reasonable predictions. Wadnerkar et al. (2012) also discussed the significant differences in the magnitude of slip velocity between Gidaspow’s (1994) model and Brucato’s drag model (Brucato et al. 1998) in the impeller zone and reported underprediction of slip velocities using both the models. Recently, Sardeshpande et al. (2010) has simulated dimensionless axial slip velocity \( V_{slip}/U_{tip} \) for 1% and 7% (v/v) solid loadings in a stirred vessel. They indicated that drag correlations proposed by Brucato et al. (1998) and Khopkar et al. (2006) overpredicted experimental axial slip velocity data in the vicinity of impeller region. Therefore, it was more appropriate to measure local slip velocity in solid-liquid stirred tanks and use these data to evaluate different interphase drag correlations.

5 Particle collision

Particle collision defines the agglomeration and/or breakup of particles in systems. This may involve a continuous phase and one or more dispersed phases. Particle collision plays a vital role in multiphase turbulent flows especially turbulent solid-liquid flows as it controls/influenced by the process.

Formulation of the collision process starts very simply, chosen for their mathematical convenience until highly involved models are obtained that can analyze complex fluid-particle interactions. The practical investigation of particle collision is difficult and problem arises as the complexity of the carrier fluid flow field rises, i.e., in turbulent flows. Table 4 lists the main particle collision models, which are discussed in the following.

The boundaries of the particle collision in turbulent flow regimes were fairly well determined in the formulations of Saffman and Turner (1956) and Abrahamson (1975). The former considered particles that were remarkably smaller than the smallest scale of turbulence and represented velocities that were perfectly correlated with the surrounding continuous phase, while the latter applied to particles with significantly high inertias, representing velocities that are entirely decorrelated from that of the continuous phase.

The collision models have been considerably improved and validated over the entire range of particle inertias by Williams and Crane (1983) and Kruis and Kusters (1997). The expression of Williams and Crane investigated the fluctuating relative motion of two liquid drops or solid particles with intermediate sizes in a turbulent gaseous system that exhibits velocities that are neither well correlated nor completely independent. Hence, this model is not applicable in solid-liquid systems. Furthermore, it is erroneously based on a cylindrical as opposed to a spherical formulation.

Yuu (1984) expressed a formulation for the fluctuating relative velocity of two inertial particles in viscous systems that are subrange of turbulence. This expression involved the added mass effect experienced by particles in turbulent liquid systems. However, it is not applicable for very small particles. Neither the model of Yuu (1984) nor that of Williams and Crane (1983) is valid for liquid systems with particle sizes in the inertial subrange of turbulence.

Kruis and Kusters (1997) derived a universal formulation for the collision kernel, which included the added mass effect. This makes the expression valid for both the viscous as well as the inertial subrange of turbulence.

Meanwhile, Hu and Mei (1997) stated that the collisions between identical particle expressions have been ignored in all previous formulations. Considering the collision between moderately inertial particles, Hu and Mei (1997) derived an expression; however, the effect of gravity was not included in their formulation. The Hu and Mei (1997) model was extended by Wang et al. (1998) considering a finite density-ratio correction as well as gravity effects.

The preferential concentration of particles, in regions of low vorticity and high strain rate, exhibited relaxation times close to the Kolmogorov time scale. Increased collision frequency range from one to two orders of magnitude is observed. Considering the effect of preferential concentration, attempts at formulating a collision kernel was initiated primarily by Sundaram and Collins (1997), who
Table 4  Collision models.

<table>
<thead>
<tr>
<th>Model</th>
<th>Comments</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \beta = \frac{8\pi}{15} (r+\tau)^3 \left( \frac{\nu}{v} \right)^{1/2} ]</td>
<td>– Valid for Gaussian, isotropic turbulence flow regimes</td>
<td>Saffman and Turner 1956</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ \beta = \sqrt{8\pi (r+\tau)^3} \left( \frac{1}{\rho_i} \right)^2 \left( \frac{D\nu}{Dt} \right)^2 \left( \tau_{ij} \right)^2 r_{ij} \left( \frac{\rho}{\rho_i} \right)^2 + \frac{2}{3} \left( \frac{\rho}{\rho_i} \right)^2 \left( \frac{r+\tau}{\nu} \right)^2 \left( \frac{D\nu}{Dt} \right)^2 \left( \tau_{ij} \right)^2 r_{ij} ]</td>
<td>– Valid as long as the particles remain in the Stokes flow regime</td>
<td>Saffman and Turner 1956</td>
</tr>
<tr>
<td></td>
<td>– Underprediction for small particle sizes</td>
<td></td>
</tr>
<tr>
<td>[ \beta = \frac{8\pi}{3} (r+\tau)^3 \sqrt{3} \left( \frac{w}{w} \right)^2 ]</td>
<td>– Overestimation by about 20% for a simple uniform shear flow and by 25% in isotropic turbulence</td>
<td>Abrahamson 1975</td>
</tr>
<tr>
<td>[ \beta = 2\pi (r+\tau)^3 \left( \frac{2}{15\pi} \right)^2 \left( \frac{D\nu}{Dt} \right)^2 ]</td>
<td>– Valid for particles with completely uncorrelated velocities</td>
<td>Williams and Crane 1983</td>
</tr>
<tr>
<td></td>
<td>– Valid for monodisperse heavy particles in an isotropic turbulent flow in the absence of global shear and gravity</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Overpredicts the collision kernel</td>
<td></td>
</tr>
<tr>
<td>[ \beta = \frac{8\pi}{3} (r+\tau)^3 \sqrt{3} \left( \frac{w}{w} \right)^2 ]</td>
<td>– Only accelerative or inertial effects included in this formulation, with no provision being made for turbulent shear effects</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– 1D formulation with isotropy assumption</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Invalid for liquid systems with particle sizes in the inertial subrange of turbulence</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Not included the added mass caused by particles moving</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Particle drag based on Stokes flow and thus places a limit on the maximum particle size</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Invalid for particle sizes in the inertial subrange of turbulence</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Underpredicts the normalized collision kernel</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Invalid for liquid systems with particle sizes in the inertial subrange of turbulence.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Improved version of the formulation of Saffman and Turner (1956)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Valid for the collision between moderately inertial particles</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Effect of gravity not included</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Added mass effects not included</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Invalid for systems including nonuniform particle concentration due to flow-particle microstructure interaction</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Invalid for small particles as the exponential as opposed to the parabolic form of the Langrangian correlation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Does not include the influence of nonuniform particle concentration due to flow-particle microstructure interaction</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– An improved version of Saffman and Turner (1956) formulation</td>
<td></td>
</tr>
<tr>
<td></td>
<td>– Invalid for inertial and viscous subrange of turbulence</td>
<td></td>
</tr>
<tr>
<td>Model</td>
<td>Comments</td>
<td>References</td>
</tr>
<tr>
<td>-------</td>
<td>----------</td>
<td>------------</td>
</tr>
</tbody>
</table>
| $\beta = \sqrt{8\pi (r_i + r_f)^3 \langle w_{\text{accel}}^2 \rangle^{1/2} \langle w_{\text{decel}}^2 \rangle^{1/2}}$ | - Included the added mass effect  
- Valid for inertial and viscous subrange of turbulence  
- On the basis of Williams and Crane (1983) for larger particles and Yuu (1984) for small particles  
- However, is not universal since there is no single expression that holds for both large and small particles  
- Underpredicts the normalized collision kernel | Kruis and Kusters 1997 |
| $\beta = 2\sqrt{2\pi (r_i + r_f)^3} \left\{ \frac{1}{15\pi} \left( \frac{r_i + r_f}{v} \right)^{3/2} + \frac{2}{8} \lambda^2 \right\}$ | - Improved version of Hu and Mei (1997) to include gravity and finite density-ratio correction  
- Invalid for systems including nonuniform particle concentration due to flow-particle microstructure interaction  
- Valid for dilute concentration systems | Wang et al. 1998 |

Zhou et al. 2001

Wang et al. 2000

Zaichik et al. 2006

Zaichik et al. 2006

---

(Table 4 Continued)
used radial distribution function at contact to account for the relative velocity PDF and the concentration effect for the decorrelation of adjacent particle motion.

The collision kernel by Sundaram and Collins (1997) was based on a cylindrical formulation that was later considered erroneous, and therefore, Wang et al. (2000) corrected it using a spherical approach.

The improved model allowed Wang et al. (2000) to isolate the effect of turbulent transport from the preferential or accumulation concentration effect as quantified by the radial distribution function. Afterward, Zhou et al. (2001) extended Wang’s model to include bidisperse as opposed to monodisperse particles.

However, the mentioned models are all based on collision data obtained through DNS. Different limitations arise from the numerical simulation on the magnitude of the Reynolds number. Therefore, the effect thereof on the collision process in turbulent flow remains elusive.

Moving away from DNS, several researchers (Alipchenkov and Zaichik 2003, Zaichik and Alipchenkov 2003, Zaichik et al. 2006) succeeded to model accumulation of inertial particles and binary dispersion in an isotropic turbulent flow field through a kinetic equation for the PDF of the relative velocity of a pair of particles. In conclusion, numerical modeling of the collision process has the advantage of higher accuracy and ability to control the primary variables.

6 Suspension quality

The aim of the equations and relations mentioned above is to investigate the quality of solid suspension, which can be quantified through some important criteria including drawdown of floating solids, just off-bottom suspension \( N_{j_{b}} \), suspension height, complete suspension, and homogeneous suspension (Ochieng and Lewis 2006b).

6.1 Drawdown of floating solids

Generally, particle flotation depends on three different phenomena: i) surface tension effects and poor wettability, causing the surface tension force to be greater than the gravitation force; ii) powders with low bulk density, which tend to agglomerate and trap air; and iii) low true density, whereas flotation is caused by buoyancy force (Waghmare et al. 2011).

Drawdown of particles in stirred vessels happens when the downward forces (turbulence and drag) overcome the upward forces (buoyancy and the surface tension) when the impeller is turned on, which is shown in Figure 1. Generally, CFD simulations clarify three mechanisms of solid drawdown: mean drag, turbulent fluctuations, and single vortex formation. In the first mechanism, large waves and swirls break up stagnant zones and ingest solids. Besides, some macro-instabilities are produced over the entire free surface of liquid initially. They also lead to breakage of solid clumps and assist distribution of particles in strong liquid circulation. In this mechanism, the particle slip velocity should be lower than the axial component of the near surface of liquid. In the second mechanism, energetic surface eddies along with the splashy and wavy surface pull the solids down. In this mechanism, very large eddies tend to be oriented against the mean circulation loops and eddies smaller than the particles are not able to draw down particles due to energy deficiency. Generally, eddies that are 3–10 times larger than the particle are more applicable in this mechanism. The last mechanism is applicable for nonbaffled stirred vessels. In these systems, large stable vortex is produced at the center of liquid bulk and breaks up stagnant regions at the surface. Therefore, the centrifugal forces pull the solid particles to the vortex surface. The best solid distribution in this mechanism has been found in systems with one single baffle. However, particles still tend to concentrate around the vortex.

Khazam and Kresta (2008) investigated the interactions between impeller and tank geometry by flow visualization as well as CFD simulations. They investigated one axial and two mixed flows over a solid concentration range of 2–10 vol%. They found that a stable central vortex acted as a centrifuge to concentrate a layer of solids close to the liquid surface. Multiple reference frames (MRFs) were used in their study, which were suitable for both the down-pumping pitched blade turbine and the up-pumping pitched blade turbine. This selection was due to the strong momentum exchange between the whole bulk and impeller zone (Sajjadi et al. 2012). In the same study, turbulence and flow were predicted more accurately via
LES model within a long simulation time (1 month). The $k$-$\varepsilon$ model decreased the simulation time to about 1 h, but there was an underprediction due to overcalculation of diffusive term.

In CFD simulation of fully baffled systems, the fluctuation of free surface is negligible. However, the medium-scale transient eddies and the behavior of surface turbulence in the system containing one singular baffle should be considered. In the study of Khazam and Kresta (2008), CFD simulation showed similar behavior for large changes in turbulence and mean flow in single phase with and without existence of solid particles. This observation was also independent of particle concentration. This assumption (or observation) was confirmed by Montante et al. (2001a,b).

Recently, Waghmare et al. (2011) simulated solid drawdown phenomenon in nonstandard tanks with different geometries, which included tilted shaft, nonstandard impellers, as well as multiple impellers, and developed a scale-up correlation using CFD. Their correlation was based on fundamental hydrodynamic parameter, velocity, and operating parameters. The goal was to calculate residence time of particles on the liquid surface. They used two important assumptions: i) the surface of the liquid was a thin layer of liquid at the top of the tank without adversely affecting the quality of the grid and ii) the distortion of free liquid surface was negligible; hence, free surface was treated as symmetry boundary. The movement of inert solid particles was simulated using discrete phase modeling. This model assumes only one-way coupling between liquid and solid and performs Lagrangian tracking of particles. The drawdown rate also depends on solid properties such as particle density, diameter, particle-particle interactions (stickiness), and particle-liquid interaction (wettability). The results of the developed CFD were accurate, but the correlation failed to predict drawdown rate for cases with strong vortex formation. The authors also found the second mechanism to be dominant for cases with low submergence. However, the correlation based on mean drag showed satisfactory agreement with the experimental data.

6.2 Off-bottom solid suspension and complete suspension

There are two other main operational requirements for investigating solid suspension in stirred vessels, which are critical impeller speed for $N_j$ and critical impeller speed for just complete suspension ($N_j^\infty$) (Armenante and Nagamine 1998). $N_j$ causes particles to just suspend from the bottom of the vessel completely and not stay stationary at the bottom for more than 1–2 s. It is also dependent on the ratio of the impeller diameter to vessel diameter and impeller clearance. Optimum stirrer velocity is required for obtaining complete off-bottom suspension and uniform dispersion in mixing operation. The impeller speed must not be too high in order to allow for an acceptable energy consumption, and it is very important for solid slurrying, efficient mass transfer, industrial mixing process optimization, and design (Abu-Farah et al. 2010). CFD simulation can produce accurate prediction of $N_j$, Table 5 shows the prediction models for off-bottom suspension.

Kee and Tan (2002) introduced a new CFD approach for prediction of minimum impeller speed by observation of transient profiles of the solid phase volume fraction for the layer of cells adjacent to the bottom of the vessel. They also characterized the effect of $C$ and $D$ on $N_j$.

Ochieng and Lewis (2006b) provided quantitative and qualitative insight into solid suspension by investigating the results of CFD and laser Doppler velocimetry. They used three different criteria to investigate $N_j$, based on CFD simulation results. They also indicated that transient simulation produced more accurate results than steady simulation did. Besides, CFD produced better results of cloud height and off-bottom suspension for low solid loading (<6%) and small particles ($d_p < 150$ μm).

Murthy et al. (2007) studied the influence of geometrical parameters on critical impeller speed in both solid-liquid and gas-solid-liquid systems. The work covered solid loading from 0.34 to 15 wt%. They further investigated the effect of particle size and solid loading. They confirmed that for a fixed set of operational conditions and constant configuration of impeller and tank, the uniformity of solids decreased with an increase in diameter of particle. They could predict the effect of solid loading on liquid velocity successfully using CFD simulation.

Lea (2009) focused on a similar problem in a system containing dense solid-liquid interaction. They developed a design heuristic that can be useful in industrial processes.

The study of Micheletti et al. (2003) is noteworthy in order to further clarify the importance of this parameter. Micheletti et al. (2003) found that the liquid phase mixing process showed a complex interaction with suspension quality and fluid mixing in stirred slurry reactors with high solid loading. Meanwhile, the trend of the mixing time depends on the impeller rotational speed and suspension quality. So, mixing time for incomplete suspension regime increased until a maximum value was achieved and gradually decreased with higher impeller speed until the $N_j^\infty$ condition (Micheletti et al. 2003). Kasat et al. (2008) also
Table 5 Prediction models of off-bottom suspension.

<table>
<thead>
<tr>
<th>Assumptions and remarks</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_{js} = \left( \frac{g \Delta \rho}{\rho_l \rho_p} \right)^{0.5} \frac{d_p^{0.8} T}{\rho_l^{0.58} \rho_p^{0.39} D^{1.25}}$</td>
<td>Basic assumption:</td>
</tr>
<tr>
<td>- Based on the transferred kinetic energy of turbulent eddies to the particles and the potential energy gained by the particle</td>
<td></td>
</tr>
<tr>
<td>- Cannot justify the higher effectiveness of the impeller that creates mass circulations than that of creates a lot of turbulence</td>
<td></td>
</tr>
<tr>
<td>- Cannot consider the effect of solid concentration and viscosity</td>
<td>Baldi et al. 1978</td>
</tr>
<tr>
<td>$N_{js} = \left( \frac{g \Delta \rho}{\rho_l \rho_p} \right)^{0.5} \frac{d_p^{0.8} T}{\rho_l^{0.58} \rho_p^{0.39} D^{1.25}}$</td>
<td>Based on the balance between the downward and upward forces acting on particles</td>
</tr>
<tr>
<td>- Cannot justify the assumption of homogenous distribution of particles nor than no slip condition between solid and liquid</td>
<td></td>
</tr>
<tr>
<td>- Applicable just for very diluted solid concentrations</td>
<td>Narayanan et al. 1969</td>
</tr>
<tr>
<td>$N_{js} = \left( \frac{g \Delta \rho}{\rho_l \rho_p} \right)^{0.5} \frac{d_p^{0.8} T}{\rho_l^{0.58} \rho_p^{0.39} D^{1.25}}$</td>
<td>Based on the Baldi energy balance with paying attention to eddy sizes</td>
</tr>
<tr>
<td>- Cannot justify the higher effectiveness of the impeller that creates mass circulations than one that creates a lot of turbulence</td>
<td></td>
</tr>
<tr>
<td>- Cannot consider the effect of solid concentration and viscosity</td>
<td>Rieger and Ditl 1994</td>
</tr>
<tr>
<td>$N_{js} = \left( \frac{g \Delta \rho}{\rho_l \rho_p} \right)^{0.5} \frac{d_p^{0.8} T}{\rho_l^{0.58} \rho_p^{0.39} D^{1.25}}$</td>
<td>Based on the forces acting on particles and liquid velocity near the bottom of the vessel incipient motion of particles</td>
</tr>
<tr>
<td>- Cannot justify the arrangement parameters of solid particles</td>
<td>Shamlou and Zolfagharian 1987, Mak 1992</td>
</tr>
<tr>
<td>Fine particle ($Ar \leq 40$)</td>
<td>Based on the Archimedes number via two mechanisms</td>
</tr>
<tr>
<td>$N_{js} = \left( \frac{g \Delta \rho}{\rho_l \rho_p} \right)^{0.5} \frac{d_p^{0.8} T}{\rho_l^{0.58} \rho_p^{0.39} D^{1.25}}$</td>
<td>First, complete suspension of fine particles at high shear stresses of wall boundary layer</td>
</tr>
<tr>
<td>- Second, based on the analysis of the pump characteristics of a stirred vessel</td>
<td></td>
</tr>
<tr>
<td>- Requires accurate prediction of shear rate at the boundary layer of the agitated tank</td>
<td>Molerus and Latzel 1987</td>
</tr>
<tr>
<td>Coarse particles ($Ar &gt; 40$)</td>
<td>Based on the difference between the liquid velocity and terminal settling velocity of particle</td>
</tr>
<tr>
<td>$N_{js} = \left( \frac{g \Delta \rho}{\rho_l \rho_p} \right)^{0.5} \frac{d_p^{0.8} T}{\rho_l^{0.58} \rho_p^{0.39} D^{1.25}}$</td>
<td>Velocity characterization calculated by measuring actual values of shear rate</td>
</tr>
<tr>
<td>- Prediction of $N_{js}$ based on the ratio between settling velocity and $N_{js}$</td>
<td>Wichterle 1988</td>
</tr>
<tr>
<td>$N_{js} = \left( \frac{g \Delta \rho}{\rho_l \rho_p} \right)^{0.5} \frac{d_p^{0.8} T}{\rho_l^{0.58} \rho_p^{0.39} D^{1.25}}$</td>
<td>Power input dissipated by two phenomena: consumption of power to avoid settling and generating discharge flow for suspension</td>
</tr>
<tr>
<td>- Inaccurate prediction of fluctuating velocity at the bottom of the vessel that led to under prediction of $N_{js}$</td>
<td>Mersmann et al. 1998</td>
</tr>
</tbody>
</table>
reported similar observations while using CFD to investigate complex interactions between suspension quality and fluid mixing. They reported the maxima in mixing time, which was nearly 10 times of the minimum value at $N=5$, $rps=13N_{CS}$. The delayed mixing in the top clear liquid was due to very low liquid velocities in this section and was responsible for the increase in mixing time.

Recently, Fletcher and Brown (2013) used two different CFD approaches to study solid suspension, which were E-E and algebraic slip modeling. Both of these approaches provided computationally efficient results. The authors further investigated the importance of turbulent dispersion forces and the role of turbulence model (homogeneous or phasic). Both of these produced similar results, but there was less solid dispersion in the homogeneous case.

Prediction methods of $N_{js}$ through CFD can be classified into five groups: tangent-intersection method, particle axial velocity method, transient profile method, variation of particle concentration, and Zwietering (1958) correlation.

### 6.2.1 Tangent-intersection method

This method was proposed by Mak (1992) and could be applied both experimentally and computationally:

$$N_{js} = S \left( \frac{g \Delta \rho}{\rho_t} \right)^{0.65} \left( \frac{d_p^{0.31} \rho_t^{0.2} v^{0.1}}{D^{0.85}} \right).$$  \hspace{1cm} (8)

where $S$ is constant for a given system geometry, $\Delta \rho = \rho_s - \rho_l$. In this method, a horizontal plane is assumed with a small displacement from the tank bottom. The distance from the tank bottom for measurement of particle concentration is arbitrary. Then, mean particle concentration is plotted versus impeller speed at this height. $N_{js}$ can be identified from the tangents to this curve drawn at the points having minimum and maximum slopes. Hosseini et al. (2010) employed this method to investigate $N_{js}$ and reported satisfactory agreement between the CFD and experimental data. However, Tamburini et al. (2011) reported that transient profile provided a strong overestimation of $N_{js}$ for all investigated systems.

### 6.2.2 Particle axial velocity method

Wang et al. (2004) employed a method based on axial velocity of solid phase in the computational cells near the tank bottom at different impeller speeds. Based on this method, all particles are considered to be suspended when the axial velocity of the solid phase in some cells becomes positive. These cells are located at areas where it is difficult to suspend the solid particles. Wang et al. (2004) made the position the locus of accumulation for the last particles to be suspended, since the main flow was from the periphery towards the center at the bottom of the tank.

Ochieng and Lewis (2006b) proposed a CFD simulation method to determine $N_{js}$ in a flat-bottomed tank using high solid loading. In their method, the simulation was initiated with settled particles at the vessel bottom and they found that drag curves and turbulence models were the most important factors for estimation accuracy.

### 6.2.3 Transient volume fraction profile method

Kee and Tan (2002) adopted a method based on solid transient volume fraction profile in a 2D transient simulation. They proposed two criteria to identify $N_{js}$ at different impeller speeds. First, all transient volume fraction profiles versus time exhibited steady-state behavior; second, all steady-state values of volume fraction were approximately 50% of the initial packed volume fraction. These criteria were used because all solid particles are entrained and circulated in the continuous phase at complete suspension state, so the volume fraction profiles of cells at the tank bottom would eventually attain steady-state behavior. Tamburini et al. (2011) reported that transient profile provided a strong overestimation of $N_{js}$ for all investigated systems.

### 6.2.4 Variation of particle concentration

A method was proposed by Wang et al. (2004) to monitor the variation in particle concentration versus impeller speed. In this method, complete off-bottom suspension was considered achieved when solid volume fraction at the place where the last particle was suspended showed some values lower than the maximum value. However, the definition of the exact volume fraction corresponding to complete suspension is subjective.

### 6.2.5 Applying Zwietering correlation in CFD simulation

Zwietering correlation in CFD simulation is the other method. The basic correlation was developed by Zwietering (1958), and most of the recent works on the critical impeller speed have been based on this correlation:

$$N_{js} = S D^{0.85} A,$$  \hspace{1cm} (9)
where $N_p$ depends on solid-liquid mixture properties [by geometry-dependent coefficients $A$, Eq. (7)] and vessel geometry (by coefficient $S$):

\[ A = v^{0.1} d_p^{0.2} \left( \frac{g (\rho_s - \rho_l)}{\rho_l} \right)^{0.45} w_s^{0.11}. \]  

(10)

In this equation, $v$ is liquid kinematic viscosity, $d_p$ is particle diameter, $\rho$ is density, and $w$ is defined as

\[ w_s = \frac{\rho_s \alpha_s}{\rho_l (1 - \alpha_s) + \rho_s \alpha_s}, \]  

(11)

where $\alpha$ is the solid volume fraction.

Ochieng and Lewis (2006b) estimated just-suspended speed and cloud height using the Zwietering (1958) model and Bittorf and Kresta (2003) correlation, respectively. They employed a Eulerian-based multiphase approach along with MRF approach to provide an initial flow field for fully predictive sliding grid (SG) to investigate off-bottom suspension of nickel solids and cloud height in a stirred reactor. However, Zwietering (1958) correlation is rarely used in E-E simulation because of its complexity. Derksen (2003) employed this model using the EL approach along with LES. In this simulation, 6.7 million particles were tracked in a liquid flow field. It was proposed that a realistic particle distribution throughout the tank could be obtained by considering particle-particle collisions. The collision algorithm was improved to reach this aim because it inhibited particles to be at mutual distance smaller than the particle diameter. The CFD simulation underpredicted $N_p$, especially for larger particles ($d_p > 150$ μm), and this disparity was attributed to the drag force, which decreased with an increase in surface. For larger particles ($d_p > 300$ μm), the deviation was 6%. The simulation was also in excellent agreement with the experimental results for solid loading up to 10%, but this model failed to show the cloud height for higher loading rate. This was attributed to empirical constants that were used in the formula (such as $k-e$, drag curves, nondrag forces, and solid pressure). The author explained that CFD simulation yielded the best result for smaller particles along with low loading rate.

Suspension curves show the amount of suspended solids and power consumption at different impeller speeds, including the partial ($N < N_p$) or complete ($N > N_p$) suspension conditions. Tamburini et al. (2011) developed an original CFD modeling approach with the aim of numerically predicting suspension curves with two different types of experimental data (Pressure Gauge Technique and snapshot data) for validation. They implemented a posteriori algorithm, namely, excess solid volume correction with an iterative approach for particle bed lying at the bottom to describe all partial suspension regimes. The best results came from modeling employing asymmetric $k-e$ for turbulence and standard drag model with two-way coupling without any additional term arising from turbulence closure in continuity equations. Zwietering (1958) also offered another method that could be used for this purpose.

6.3 Cloud height

Another criterion that provides a qualitative indication of suspension quality is height of homogeneous zone. However, it cannot consider local mixing quality and provides only satisfactory information on a global parameter. The height of homogeneous zone is also called cloud height. Mixing is vigorous below this interface but limited above this interface (in clear volume), which results in increased mixing time and large amount of unreacted fluid in this area. Several authors have simulated solid distribution in mixing systems to investigate this parameter. However, most of the published works focused on 1D sedimentation of particles, resulting in a function based on Peclet number. The solid concentration was $<6$ wt%, whereas no well-defined interface was formed. At concentration above $10$ wt%, clear interface was formed at the place where the upward and downward velocity balance each other.

Stratified flow, hindered settling, negatively buoyant jets, and solid iso-surface are four available phenomena to investigate the formation of this interface. The difference between unconfined and confined flows is established by an examination of literature on stratified flows. Hindered settling happens in confined 1D flows with high solid concentration, where the presence of particles significantly reduces the area available for flow and increases particle-particle collisions. These collisions may increase drag force on the particles. Since flow in stirred tank is 3D, hindered settling models cannot truly predict solid flow.

In stirred vessels, a negatively buoyant jet penetrates upward. As the upward jet expands, velocity decreases. Meanwhile, the heavier fluid in the upward jet stops and returns to the bottom of the vessel. Negatively buoyant jets flow to a maximum height during the initial period and then drop to a lower steady-state height due to the downward drag on the free jet, refer to Figure 2. The penetration height depends on the momentum flux and buoyancy flux. Generally, three criteria are required for forming a clear interface: first, sufficient density difference, which
is provided at high solid concentration; second, momentum, which causes break up of a stratified layer; and third, additional momentum of wall jet, which results in higher penetration of jet. Therefore, jet penetration increases by increasing the momentum of wall jet. This leads to full suspension at higher impeller speed. Larson and Jonsson (1994) indicated that increasing jet nozzle speed in a two-layer stratified fluid increased the penetration distance of jet into the second layer. This is similar to the stirred tank where an increase in impeller speed raises the interface height, which may result in fully suspended situation. Any additional momentum in the wall jet increases the penetration height. This behavior proposes a mechanism for formation of cloud height. In other words, the location of clear interface can be estimated by this technique if the particle distribution is driven by upward jet. Bittorf and Kresta (2001) showed that the flow at the wall of a stirred vessel containing axial impellers could be characterized using four 3D wall jets in front of each baffle.

In another work, Bittorf and Kresta (2003) modeled this technique by CFD simulation. They defined an interface at the location where the upward velocity of fluid at the wall was exactly balanced by the downward velocity of particles. Their model was based on the relation between the maximum velocity in wall jet and solid cloud height, which is the flow created when fluid is blown tangentially along a wall. The authors assumed that once particles were lifted and prevented from settling, a force depending on the wall jet must move them away from the bottom. Their model assumed that the cloud height was determined only by mean flow conditions, not turbulence or macro-instabilities. The mean flow can also be described by 3D wall jet model introduced previously. However, wall jet model in stirred tanks is sensitive to geometry. This criterion was clarified by Bittorf and Kresta (2003). Other authors (Hicks et al. 1997, Bujalski et al. 1999) have reported data for solid distribution and cloud height in a form suitable for model development based on wall jets. Hicks et al. (1997) examined cloud height with different solid types with constant concentration. Bujalski et al. (1999) also varied the solid concentrations (20–40 wt%). Satisfactory agreement between the CFD and experimental result was observed in both studies. This technique has also been successfully applied by Ochieng and Lewis (2006b). An excellent agreement between the modeled and the experimental data for solid loading up to 10% was reported in their study. However, a poor prediction was obtained for higher solid loading. The authors attributed this deviation to some factors. First, the $k$-$\varepsilon$ model is more applicable in simple systems compared to high-solid-containing systems. Second is the density difference between the models developed by Bittorf and Kresta (2003) and Ochieng and Lewis (2006b). Third is the higher interaction between solid particles in the system and effect of drag and nondrag forces, which depends on the particle interactions. The solid interface method was introduced by Kasat et al. (2008). The cloud height in this method was defined as the maximum vertical coordinate of a solid iso-surface. The location of this iso-surface was defined as the average of solid phase volume fraction. Grétarsson et al. (2012) also applied this method in E-G approach and found reasonable predictions. Micale et al. (2004) used the opposite direction of the last model to find the solid cloud height. They used the location of particle-free liquid layer to find the solid suspension height. However, they obtained poor prediction results. Recently, Wadnerkar et al. (2012) have also used this method to investigate cloud height and reported satisfactory agreement. In CFD simulation, most of the other works in this area have focused on comparing the experimental data with the simulation results using different frame grids (MRF or SG), approaches, turbulence models, or drag models (Montante et al. 2001b, Kee and Tan 2002, Derksen 2003).

### 6.4 Solid distribution

Uniformity of a multiphase system is another important parameter especially in mass transfer. This criterion can be determined by investigating solids concentration distribution in the entire vessel.
6.4.1 Settling velocity model

In this context, polydisperse approach is one of the emerging multiphase simulation concepts to visualize particles of a specific size range in systems with high solid holdup (Sharma and Shaikh 2003, Ochieng and Lewis 2006b). The first attempt by Magelli et al. (1990) evaluated dispersed phase behavior using terminal settling velocity and mass balance. The continuous phase was obtained by 1D axial dispersion model. A more common procedure was to assume a single-phase flow field for the continuous phase as a basis for the dispersed phase calculations. It was clear that there was no coupling back from the dispersed to the continuous phase in this procedure. Smith (1997) used this approach to calculate Lagrangian particle tracks. Brucato et al. (1996, 1997) used single-phase results for the continuous phase as initial data for their Settling Velocity Model along with E-E approaches in two separate investigations containing single and multiple impeller systems. They focused on the calculation of a solid concentration profile based on the mass balance of each control volume. A similar method was employed by Myers et al. (1995) and Bakker et al. (1994). They introduced a term of turbulent dispersion calculation for dispersed phase into a continuity equation and assumed a constant slip equal to terminal settling velocity for obtaining the dispersed phase velocities. Decker and Sommerfeld (1996) and Barrue et al. (1997) introduced two-way coupled 3D E-L calculations accounting for particle turbulent dispersion through instantaneous fluid velocity that acts on a particle at a certain time. Hamill et al. (1995) introduced a full two-way coupled calculation along with multifluid E-E approach on a propeller stirred crystallizer. It was challenging to conduct measurements and modeling using such systems, especially with high solid loading, even with a variety of simplifications.

Recently, Klenov and Noskov (2011) simulated this model to study solid distribution in liquid-solid stirred vessel equipped with five impellers mounted on a single shaft, which created four separated domains in the reactor with 3D complex swirling streams. They observed parameters such as specific density of solid phase and place of solid injection and found these to be very influential on the distribution of solid suspension in the slurry reactor. The mechanical energy of a revolving impeller transforms to energy of turbulent rotation flow and then the turbulence energy dissipates through small-scale curls. They also observed minimal nonuniformity of axial distribution for high-density solid particles. They used correlation for settling velocity in stirred tank and still liquid to estimate the order of magnitude of solid settling velocities (Pinelli et al. 2009).

6.4.2 Standard deviation model

Bohnet and Niesmak (1980) presented the most widely used criteria that quantified suspension quality in stirred vessels by means of standard deviation. This method was based on a standard deviation, which was suitable to be used with the E-E approach, although standard deviation reduced with increment of homogenization degree:

\[
\sigma = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left( \frac{\alpha_{i,j} - \alpha_{i,avg}}{\alpha_{i,avg}} \right)^2},
\]

(12)

where \( n \) is the number of sampling locations used for allocating the solid volume fraction. On the basis of standard deviation, three ranges of suspension quality are identified. For nonuniform (incomplete) suspensions, the value of standard deviation is found to be more than 0.8. The value of standard deviation was between 0.2 and 0.8 (0.2 < \( \sigma < 0.8 \)) for \( N_{ps} \) condition and \( \sigma < 0.2 \) for homogeneous condition.

Khopkar et al. (2006) used this method along with the modified Brucato model (Brucato et al. 1998) to simulate turbulent solid-liquid flow in a stirred vessel. They observed reasonable agreement between the modeled data and the experimental data for \( N_{ps} \) critical impeller speed, and cloud height. The same methodology was successfully employed by Oshinowo and Bakker (2002). However, Montante et al. (2003) reported that \( \sigma \) varied with operational conditions, fluid properties, and tank configurations, although it lacked physical significance.

Recently, Wang et al. (2010) used this method along with the Syamlal-O’Brien-symmetric drag force model (Syamlal 1987) of the interphase momentum transfer between two dispersed solid phases and predicted solid concentration in different sections of stirred vessel.

6.4.3 Size-dependent model

Modeling of size-dependent classification function in CFD was done by Sha et al. (2001) through a Eulerian simulation approach to model six phases of solid particles using the following model:

\[
n_p = \frac{n_s}{f(L)h(Z_s,f(N,D),L)} \times \exp\left[ \frac{1}{G_f} \int_{f(L)h(Z_s,f(N,D),L)}^{l} \frac{dL}{f(L)h(Z_s,f(N,D),L)} \right].
\]

(13)

However, there was very little comparison between the simulation results with the experimental data even
though this aspect is crucial for validating the adopted models and procedures (Sha et al. 2001). In another work by Sha and Palosaaari (2002), they used the model to estimate the population-density distribution and simulation of local particle size distribution in a crystallizer with imperfect mixed suspension. They calculated the classification by population density and suspension density based on the volume fraction in each cell with the CFD program successfully. Ochieng and Lewis (2006b) employed the fully predictive Eulerian simulation to investigate the effect of solid loading and particle size on solid distribution in a stirred vessel containing high-density particles (nickel). They reported that high-density particles tend to settle at the bottom of the tank so particle density affects particle size distribution in both the radial and axial directions, and assumption of mono-disperse-particle may result in incorrect prediction. However, they validated the modeling approach only for monodispersed solid fractions and dilute conditions.

Špidla et al. (2005) measured axial and radial particle concentration gradient for a solid-liquid suspension (with average particle concentration of 5 vol%) in a just-suspended state in a baffled stirred vessel equipped with pitched blade turbine. They performed E-E multiphase model along with the mixture of $k$-$\varepsilon$ turbulence model (Špidla et al. 2005). They used three different drag models: Schiller-Naumann (Schiller and Naumann 1935), Pinelli (Pinelli et al. 2009), and Brucato (Brucato et al. 1998), and suggested higher drag coefficient for obtaining better results.

Wang et al. (2006) successfully simulated the distribution of dispersed oil phase under high agitation rate using the E-E multiphase method to simulate a liquid-liquid-solid system in a stirred tank. However, the method/simulation failed under low impeller speed. In another work (Wang et al. 2010), they applied CFD model to investigate a liquid-solid-solid two-phase flow field to predict distributions of two dispersed solid phases in the flow field. This was done based on the E-E multiphase approach, where they studied crystallization of monosodium aluminate hydrate from a super saturated aluminate solution containing red mud as leaching liquor of bauxite. They used two methods for their liquid-solid-dispersion system (glycerite, red mud, and sand). The first method was based on first-order upwind discretization with 245–258 K grid sizes scheme, and the second was based on the Quadratic Upstream Interpolation for Convective Kinematics discretization scheme with 690–740 K grid sizes. Within these approaches, they employed Gidaspow’s (1994) drag force and Syamlal-O’Brien-Symmetric’s drag force models for the interphase momentum exchange for liquid-solid and solid-solid, respectively. The liquid and two solid phases were all considered as different continua, interpenetrating and interacting with each other in the whole computational domain. The obtained simulation result was in good agreement with experimental results. They found that the simulated and distributions in the flow fields by the two methods were basically the same (Wang et al. 2010).

Montante and Magelli (2007) applied CFD simulation to calculate solid concentration distribution and measured flow field of all intervening phases and the vertical distribution of solid concentration by an optical technique. However, they considered only two solid fractions with equal size. They used three different sets of RANS equations: one for continuous phase and the other two for the two dispersed solid fractions. They also modeled momentum transfer between the liquid phases and each solid phase by drag forces with influence of turbulence and obtained realistic predictions of solid distribution along the vessel’s vertical coordinates.

Tamburini et al. (2009) summarized the most important published work on solid-liquid stirred vessel until 2009 in a table in their review on turbulence models. In this work, a number of relevant information after 2009 was added into the table (Table 6).

7 Conclusions

This review shows that CFD models can obtain useful results for transport phenomena and flow field in stirred vessels containing solid particles. There is a general trend toward development of CFD simulation methods to predict solid concentration distribution, particle trajectory, particle size distributions, cloud height, and minimum stirrer speed, which have traditionally been determined using experimental methods only. However, the turbulence model still remains constrained in obtaining accurate CFD simulation data especially in systems with high solid loading.

1. Generally, the review shows that the E-E approach is more popular than E-L, in spite of the momentum exchange between the operational phases due to drag and lift. Virtual mass through the interface can be modeled more accurately by E-L in comparison with E-E. This is caused by the huge demand of computational cost of E-L especially at a high dispersed phase volume fraction, where the interactions between the two phases are increased as well (Ochieng and Onyango 2010). In addition, the combination of $k$-$\varepsilon$ model with the modified Brucato model has proposed satisfying
<table>
<thead>
<tr>
<th>Authors year/year/system</th>
<th>Grid size, type, impeller motion model</th>
<th>Flow variable</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tamburini et al. 2011/2011</td>
<td>430,080 (hexahedra) for half of the tank SG, MRF, CFD code: CFX4.4 (USRIPPT)</td>
<td>Liquid free stream turbulence, radially averaged axial profile of solid volumetric fractions</td>
<td>Purpose: prediction of suspension curves Turbulence model: standard k-ε Drag: standard, Gidaspow’s dense particle, Tamburini Notes: Eulerian/Eulerian</td>
</tr>
<tr>
<td>Waghmare et al. 2011/2011</td>
<td>300,000–800,000, Hexahedral MRF, CFD Code: Fluent 6.3.26</td>
<td>Liquid surface velocity, draw down rate</td>
<td>Purpose: scaling up liquid-lightweight solids mixing Turbulence model: RNG k-ε Drag: – Notes: Eulerian/Lagrangian</td>
</tr>
<tr>
<td>Authors year/year/system</td>
<td>Grid size, type, impeller motion model</td>
<td>Flow variable</td>
<td>Remarks</td>
</tr>
<tr>
<td>--------------------------</td>
<td>--------------------------------------</td>
<td>---------------</td>
<td>---------</td>
</tr>
<tr>
<td>Wadnerkar et al. 2012/2012</td>
<td>224280 (MRF)</td>
<td>245,000–258,000 Hexahedron and tetrahedral</td>
<td>Purpose: analyzing drag models</td>
</tr>
<tr>
<td>T, D/T, C/T, N, W/T, Z/T, 0.2 m, T/3, T/3, 4, 0.1T, T</td>
<td>CFD code: ANSYS 12.1 FLUENT</td>
<td>Velocity components</td>
<td>Turbulence model: standard k-ε</td>
</tr>
<tr>
<td>Water, small glass</td>
<td>Slip velocity</td>
<td>Drag: Gidaspow, Brucato, modified Brucato drag models</td>
<td></td>
</tr>
<tr>
<td>$d_s = 0.3 \text{ mm}$</td>
<td>Turbulent kinetic energy (TKE)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\rho_s = 2550 \text{ kg}$</td>
<td>Cloud height and homogeneity</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha = 1%$, $Re = 75,071.85$, $Po = 4.950$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha = 7%$, $Re = 81,946.97$, $Po = 4.633$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wang et al. 2010/2010</td>
<td>245,000–258,000 Hexahedron and tetrahedral</td>
<td>Purpose: investigation solid suspension qualities of both liquid-solid and liquid-solid-solid systems</td>
<td></td>
</tr>
<tr>
<td>Six-bladed Rushton, 200–300</td>
<td>MRF</td>
<td>Turbulence model: RNG k-ε</td>
<td></td>
</tr>
<tr>
<td>0.14 m, T/2, 0.357T, 0, T</td>
<td>CFD code: Fluent 6.3</td>
<td>Drag: Syamlal-O’Brien-symmetric drag force model</td>
<td></td>
</tr>
<tr>
<td>Aluminate crystal</td>
<td>Mixing time</td>
<td>Notes: E-E</td>
<td></td>
</tr>
<tr>
<td>$\alpha = 1%$</td>
<td>Power number</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\rho_{ac} = 2340 \text{ kg/m}^3$</td>
<td>Row pattern</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$d_{ac} = 102 \mu\text{m}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Red Mud</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\rho_{ac} = 2242.7 \text{ kg/m}^3$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$d_{ac} = 10.7 \mu\text{m}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Qi et al. 2012/2012</td>
<td>126,928 meshes</td>
<td>Purpose:</td>
<td></td>
</tr>
<tr>
<td>Smith turbine</td>
<td>CFD code: ANSYS CFX 10.0</td>
<td>Turbulence model: standard k-ε</td>
<td></td>
</tr>
<tr>
<td>0.476, 0.4T, 4, 0.1T, T, liquid</td>
<td>Power number</td>
<td>Drag: Schiller Naumann drag</td>
<td></td>
</tr>
<tr>
<td>$M = 1 \times 10^{-3}, 2 \times 10^{-2}$</td>
<td>Row pattern</td>
<td>Notes: E-E</td>
<td></td>
</tr>
<tr>
<td>$d = 1 \times 10^{-4}, 3 \times 10^{-4}$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\rho_o = 2500–4000 \text{ kg/m}^3$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2.5–11%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tamburini et al. 2012/2012</td>
<td>245,000–258,000 Hexahedron and tetrahedral</td>
<td>Purpose: investigation of the $N_j$</td>
<td></td>
</tr>
<tr>
<td>Six-bladed Rushton turbine, 200–800</td>
<td>MRF and SG</td>
<td>Turbulence model: standard k-ε</td>
<td></td>
</tr>
<tr>
<td>0.19 m, T/2, T/3, 4, T/10, H=T</td>
<td>CFD code: CFX4.4</td>
<td>Drag: Brucato, Pinelli</td>
<td></td>
</tr>
<tr>
<td>Glass ballottini particles</td>
<td>Normalized solids volume fraction, power number, cloud height</td>
<td>Notes: E-E</td>
<td></td>
</tr>
<tr>
<td>$\rho_o = 2500 \text{ kg/m}^3$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\alpha = 16.9–33.8 \text{ wt}%$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\rho_o = 2470 \text{ kg/m}^3$</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### Table 6 (Continued)

<table>
<thead>
<tr>
<th>Authors year/year/system</th>
<th>Grid size, type, impeller motion model</th>
<th>Flow variable</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Montante et al. 2012/2012</td>
<td>126,928 meshes, MRF, CFD code: ANSYS CFX 10.0</td>
<td>Turbulence modulation and axial solid-liquid, Slip, Velocities</td>
<td>Purpose: the effect of particle properties (density and diameter) and effective slurry viscosity on particle suspension behavior</td>
</tr>
<tr>
<td>Tamburini et al. 2014</td>
<td>MRF, CFD code: ANSYS CFX 4.4</td>
<td>Axial profiles of particle concentrations</td>
<td>Purpose: influence of drag and turbulence modeling on particle suspension behavior</td>
</tr>
<tr>
<td>Tamburini et al. 2013</td>
<td>MRF, CFD code: ANSYS CFX 4.4</td>
<td>Solid volumetric fractions (radial and axial profiles), suspension curve data</td>
<td>Purpose: prediction of solid particle distribution</td>
</tr>
</tbody>
</table>
results in most cases. In the Eulerian approach, most researchers have assumed monodispersed size of particles. Ochieng and Lewis (2006b) showed that this assumption could not predict practical applications accurately especially for high-density particles.

2. Assuming standard drag coefficient (quiescent flow) results in large errors in the simulation of dispersed phase concentration profiles of a turbulent flow. Drag coefficients in turbulent fluids depend on both flow field and particle characteristics.

3. In solid suspension studies, CFD makes it possible to obtain detailed information on the flow field and simulation of off-bottom solid suspension, solid cloud height, and solid concentration distribution. Satisfactory agreement between the experimental findings and the numerical predictions has been observed.

4. In particle collision, the most recent models regarding the direct numerical solutions were in good agreement with the experimental results.

5. There are much more work that can be done at the particle scale for further understanding of the relationship between the flow field in the reactor and the physiology.

6. Majority of the CFD studies for solid-liquid stirred tanks have focused on prediction of particle suspension height in a stirred vessel or have been devoted to improved prediction of solid concentration profiles. There were not enough publications for investigation of mass and heat transfer, particle-particle and particle-impeller collisions, vortex structure, power consumption, circulation and macro-mixing times, and the distribution of turbulence quantities using CFD.

7. CFD simulation is a powerful and often indispensable tool for modeling mixing systems such as solid-liquid flows in stirred vessel, similarly true for any hydrodynamic systems. However, one of the most important aspects of this type of simulations that the computational fluid dynamicists must understand are the limitations of the methods and results need to be validated before such predictions can be relied on.

### Nomenclature

- **N**: Number of baffles
- **T**: Tank diameter, m
- **u**: Velocity vector
- **X**: Solid weight fraction

### Greek symbols

- **\( \alpha \)**: Volume fraction of disperse phase
- **\( \beta \)**: Smagorinsky eddy viscosity (\( \beta = 2/9 \))
- **\( \nu \)**: Kinematic viscosity
- **\( \rho \)**: Density
- **\( \mu(t) \)**: Turbulent viscosity, kg/m s
- **\( \mu \)**: Dynamic viscosity
- **\( \lambda \)**: Kolmogoroff length scale \( \lambda = (\nu^3/\epsilon)^{1/4} \)
- **\( \tau \)**: Stress tensor
- **\( \phi \)**: Phase hold up
- **\( \eta \)**: Scales of fluid motion
- **\( \epsilon \)**: Dissipation rate of turbulent kinetic energy
- **\( U_x \)**: Velocity components of a turbulent flow field
- **\( u_x \)**: Fluctuating velocity
- **\( E_t \)**: Total local energy dissipation
- **\( \langle u_x \rangle \)**: Mean velocity
- **\( \langle u_x^2 \rangle \)**: Mean-square velocity fluctuations
- **\( w_x^2 \) or \( \langle w_x^2 \rangle \)**: Particle root-mean-square velocity
- **\( \eta \)**: Kolmogorov microscale

### Subscripts and superscripts

- **L**: Liquid
- **S**: Solid
- **P**: Particle

### Acknowledgments:
The authors are grateful for the University of Malaya High Impact Research Grant (HIR-MOHE-D000038-16001) from the Ministry of Education Malaysia and University of Malaya Bright Spark Unit, which financially supported this work.

### References


Bionotes

Raja Shazrin Shah Raja Ehsan Shah
Faculty of Engineering, Department of Chemical Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia

Raja Shazrin Shah Raja Ehsan Shah graduated with a Chemical Engineering degree at the University of Malaya, Malaysia, in 2004 and obtained his Master’s degree from the same university in 2010. He worked in applied research for resource recovery for waste streams coming from natural rubber and palm oil industries in Malaysia, with particular emphasis on membrane technologies. In 2012, he joined the University of Malaya as a doctoral candidate working on hydrodynamic studies on multiphase systems in stirred reactors.

Baharak Sajjadi
Faculty of Engineering, Department of Chemical Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia

Baharak Sajjadi graduated with a Chemical Engineering degree at Arak University, Iran, in 2008 and obtained her Master’s degree from the same university in 2010. She worked on hydrodynamics and mass transfer investigations in airlift bioreactors with computational fluid dynamics (CFD). In 2011, she joined the University of Malaya, Malaysia, as a doctoral candidate working on biochemical processing with particular interest in biofuel production. Other interests include development, validation, and optimization in unconventional geometries.

Abdul Aziz Abdul Raman
Faculty of Engineering, Department of Chemical Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia
azizraman@um.edu.my

Abdul Aziz completed his PhD in the area of three-phase mixing. Currently, he is a professor and holds the position of Deputy Dean at the Faculty of Engineering, University of Malaya, Malaysia. His research interests are in mixing in stirred vessels and cleaner production technologies. He is also active in consultancy projects and has supervised numerous PhD candidates. He is also member of professional and learned societies such as the Institution of Chemical Engineers (IChemE, UK), Institution of Engineers Malaysia (IEM), and American Chemical Society (ACS).

Shaliza Ibrahim
Faculty of Engineering, Department of Civil Engineering, University of Malaya, 50603 Kuala Lumpur, Malaysia

Shaliza Ibrahim is attached to the Department of Civil Engineering at the University of Malaya (UM), under the Environmental Engineering Programme. A chemical engineer by training, her interest in mixing research stemmed from her PhD study back in 1988–1992 at the University of Birmingham, in the area of multiphase mixing in stirred vessels. She has been instrumental in keeping mixing research going at UM, with particular interest in solid-liquid mixing, while more recent projects are applied to biological and adsorption processes in wastewater treatment.
Graphical abstract

**Review**: This review evaluates CFD applications to analyze solid suspension quality in stirred vessels.

**Keywords**: computational fluid dynamics (CFD); drag force; solid suspension; stirred vessel.

Raja Shazrin Shah Raja Ehsan Shah, Baharak Sajjadi, Abdul Aziz Abdul Raman and Shaliza Ibrahim

Solid-liquid mixing analysis in stirred vessels

DOI 10.1515/revce-2014-0028
Rev Chem Eng 2015; xx(x): xxx–xxx