Chapter 6

CFD Simulation of Solid Suspension in Gas-Liquid-Solid Mechanically Agitated Contactor
Mechanically agitated reactors involving gas, liquid, and solid phases have been widely used in chemical industries, mineral processing industries, wastewater treatment, and biochemical industries. This is one of the most widely used unit operations because of its ability to provide excellent mixing and contact between the phases. Despite their widespread use, the design and operation of these agitated reactors remain a challenging problem because of the complexity encountered due to the three-dimensional (3D) circulating and turbulent multiphase flow in the reactor. An important consideration in the design and operation of these agitated reactors is the determination of the state of full suspension, at which point no particles reside on the vessel bottom for a long time. Such a determination is critical to enhance the performance of the reactor, because until such a condition is achieved, the total surface area of the particles is not efficiently utilized.

Hence, it is essential to determine the minimum impeller speed required for the state of complete off-bottom suspension of the solids, called the critical impeller speed. It is denoted by $N_{js}$ for solid suspension in the absence of gas and by $N_{jsg}$ for solid suspension in the presence of gas. A considerable amount of research work has been carried out to determine the critical impeller speed starting with the pioneering work of Zwietering (1958). Since then, numerous papers on determination of critical impeller speed for different operating conditions and different types of impellers have been published (Bohnet and Niesmak, 1980; Chapman et al., 1983; Kraume, 1992) for liquid–solid stirred reactors, and a few of them (Zlokarnik and Judat, 1969; Chapman et al., 1983; Warmoeskerken et al., 1984; Nienow et al., 1985; Bujalski et al., 1988; Wong et al., 1987; Frijlink et al., 1990; Rewatkar et al., 1991; Dylag and Talaga,
have been extended toward the development of correlations for the critical impeller speed for gas–liquid–solid stirred reactors.

According to the literature, in general, \( N_{js} \) is always greater than \( N_{js} \). Zlokarnik and Judat (1969) have reported that approximately 30% higher impeller speed over \( N_{js} \) is required to ensure the resuspension of solid, when gas is introduced. This is due to the reduction in impeller pumping capacity. The reason for the reduction in impeller power in three-phase agitated reactors system has been extensively studied in the literature. Chapman et al. (1983) explained the decreased liquid pumping capacity and power input on the basis of the sedimentation phenomena. Warmoeskerken et al. (1984) explained the decrease in impeller power due to the formation of gas-filled cavities behind the impeller blades. Rewatkar et al. (1991) reported that the reduction in the impeller power in the three-phase system is due to the formation of solid fillet at the center and along the periphery of the vessel bottom and the formation of gas-filled cavities behind the impeller. Table 6.1 shows the empirical correlations developed by various authors for critical impeller speed for just suspended state of solids in the presence of gas.

The critical impeller speed for gas–liquid–solid mechanically agitated reactors depend on several parameters, such as particle settling velocity, impeller design, impeller diameters and sparger design, and its location. The selection of impeller type is an important consideration for simultaneous solid suspension and gas dispersion with minimum power requirement in such reactors. In the literature, various authors (Chapman et al., 1983; Frijlink et al., 1990; Rewatkar et al., 1991; Pantula and Ahmed, 1998) have studied the performance of different types of impellers for a solid
CFD Simulation of Gas-Liquid-Solid Mechanically Agitated Contactor

suspension in a stirred tank for various ranges of operating conditions and concluded that the pitched blade turbine with downward pumping (PBTD) is more favorable at lower gassing rates and disc turbine (DT) and pitched blade turbine with upward pumping (PBTU) are more favorable at higher gassing rate.

Although the available correlations in the literature are of great importance from an operational view-point, they do not provide a clear understanding of the physics underlying the system. From a physical standpoint, the state of suspension of solid particles in the reactor is completely governed by the hydrodynamics and turbulence prevailing in the reactor. Only a few studies (Guha et al., 2007; Spidla et al., 2005; Aubin et al., 2004) have been made to understand the complex hydrodynamics of such complicated stirred reactors. Although much experimental effort has been focused on developing correlations for just-suspension speed, a systematic experimental study to characterise the solid hydrodynamics in stirred slurry reactors can hardly be found in the literature.

For this reason, computational fluid dynamics (CFD) has been promoted as a useful tool for understanding multiphase reactors (Dudukovic et al., 1999) for precise design and scale up. The RANS-based CFD approach is the most widely used approach for the multiphase phase flow simulation of such reactors. In the literature, CFD based simulations have been used to predict the critical impeller speed for a solid suspension in a liquid–solid stirred tank reactor (Bakker et al., 1994; Micale et al., 2000; Barrue et al., 2001; Sha et al., 2001; Kee and Tan, 2002; Montante and Magelli et al., 2005; Khopkar et al., 2006; Guha et al., 2008) by employing the Eulerian–Eulerian approach, and this prediction have been extended to the case of gas–liquid–solid stirred tank reactors. Recently Murthy et al. (2007) carried out CFD
simulations for three-phase stirred suspensions. The effect of tank diameter, impeller diameter, type, location, size, solid loading and superficial gas velocity on the critical impeller speed was investigated by them using the standard deviation approach. The solid loading in their study varied from 2–15% by weight. But most of the industrial applications, especially hydrometallurgical applications, involve high density particles with high concentration. Moreover, it has been reported in the literature (Khopkar et al., 2006; van der Westhuizen and Deglon, 2007) that it is difficult to quantify the critical impeller just based on the standard deviation approach alone.

<table>
<thead>
<tr>
<th>References</th>
<th>Experimental system used</th>
<th>Empirical correlation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chapman et al.(1983)</td>
<td>tank diameter = 0.29–1.83 m, impeller type = DT, PBTD and PBTU and marine propeller</td>
<td>$\Delta N_{js} = N_{js} - N_{js}$, $= kQ_{v}$ where $k=0.94$</td>
</tr>
<tr>
<td></td>
<td>impeller clearance = $T/4$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>solid loading = 0.34–50 wt %</td>
<td></td>
</tr>
<tr>
<td></td>
<td>particle density = 1050– 2900 kg /m$^3$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>particle diameter = 100–2800 $\mu$m</td>
<td></td>
</tr>
<tr>
<td></td>
<td>air flow rate = 0–32 mm/s</td>
<td></td>
</tr>
<tr>
<td></td>
<td>sparger type = ring, pipe, conical and concentric rings</td>
<td></td>
</tr>
<tr>
<td>Nienow et al.(1985)</td>
<td>tank diameter = 0.45 m, impeller type = Disc turbine</td>
<td>$\Delta N_{ji} = N_{ji} - N_{ji}$, $= kQ_{v}$ where $k=0.94$</td>
</tr>
<tr>
<td></td>
<td>impeller diameter = 0.225 m</td>
<td></td>
</tr>
<tr>
<td></td>
<td>impeller clearance = 0.1125 m</td>
<td></td>
</tr>
<tr>
<td></td>
<td>particle type = glass beads</td>
<td></td>
</tr>
<tr>
<td></td>
<td>particle diameter = 440–530 $\mu$m</td>
<td></td>
</tr>
<tr>
<td>Wong et al.(1987)</td>
<td>tank diameter = 0.29 m, impeller type = Propeller, Disc and Pitched turbine</td>
<td>$\Delta N_{ji} = N_{ji} - N_{ji}$, $= kQ_{v}$ where $k=2.03$ for DT, $k=4.95$ for PBTD</td>
</tr>
<tr>
<td></td>
<td>impeller diameter = 0.06–0.26 m</td>
<td></td>
</tr>
<tr>
<td></td>
<td>impeller clearance = 0.051– 0.076 m</td>
<td></td>
</tr>
<tr>
<td></td>
<td>particle density = 2514–8642 kg /m$^3$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>particle diameter = 200–1200 $\mu$m</td>
<td></td>
</tr>
</tbody>
</table>
**CFD Simulation of Gas-Liquid-Solid Mechanically Agitated Contactor**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value/Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air flow rate</td>
<td>0–2 vvm</td>
</tr>
<tr>
<td>Tank diameter</td>
<td>0.57–1.5 m,</td>
</tr>
<tr>
<td>Impeller type</td>
<td>RT, PBTD and PBTU</td>
</tr>
<tr>
<td>Impeller diameter</td>
<td>0.175T–0.58T m</td>
</tr>
<tr>
<td>Impeller clearance</td>
<td>T/3</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>100–2000 μm</td>
</tr>
<tr>
<td>Air flow rate</td>
<td>0–32 mm/s</td>
</tr>
<tr>
<td>Solid loading</td>
<td>0.34–50 wt %</td>
</tr>
<tr>
<td>Sparger type</td>
<td>ring, pipe, conical and concentric rings</td>
</tr>
</tbody>
</table>

\[ \Delta N_s = 132.7 V_{ss}^{0.5} D^{-1.67} T V_g \]

where \( \Delta N_s = N_{jsg} - N_{sp} \)

\( N_{sp} \) = critical impeller speed for solid suspension in the presence of sparger

\( N_{jsg} \) = critical impeller speed for suspension in gas-liquid-solid system

\( V_{ss} \) = terminal setting velocity of particle

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Dylag et al. (1994)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value/Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tank diameter</td>
<td>0.3 m and ellipsoidal bottom</td>
</tr>
<tr>
<td>Impeller type</td>
<td>DT and PBTD</td>
</tr>
<tr>
<td>Impeller clearance</td>
<td>0.5D</td>
</tr>
<tr>
<td>Particle density</td>
<td>2315 kg/m³</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>0.248–0.945 mm</td>
</tr>
<tr>
<td>Air flow rate</td>
<td>1.5–22.5 mm/s</td>
</tr>
<tr>
<td>Solid loading</td>
<td>2–30 wt %</td>
</tr>
</tbody>
</table>

For DT

\[ \frac{N_{c} D_p}{\eta g} = 18.95 \times 10^{17} \left( \frac{V_{s} D_p}{\eta g} \right)^{0.5} X^{111} \left( \frac{d}{D} \right)^{-0.33} \]

For PBTD

\[ \frac{N_{c} D_p}{\eta g} = 17.55 \times 10^{17} \left( \frac{V_{s} D_p}{\eta g} \right)^{0.5} X^{111} \left( \frac{d}{D} \right)^{-0.33} \]

Hence, the objective of this work is to carry out the CFD simulation based on the Eulerian multi-fluid approach for the prediction of the critical impeller speed for high density solid particles with solid loading in the range of 10–30% by weight. CFD Simulations were carried out using the commercial package ANSYS CFX-10. Since any CFD simulation has to be validated first, the CFD simulations have been validated with those reported in the literature (Guha et al., 2007; Spidla et al., 2005; Aubin et al., 2004) for solid–liquid and gas–liquid agitated reactors. After the validation, the CFD simulations have been extended for gas–liquid–solid mechanically agitated contactor to study the effects of impeller design, impeller speed, particle size and gas flow rate on the prediction of critical impeller speed based on both the standard deviation approach and cloud height criteria, and the simulation results were compared with our experimental results.
6.2. Experimental Methodology

The mechanically agitated contactor that was used to carry out the experiments is shown in Figure 6.1. It was a baffled cylindrical tank with an internal diameter of 250 mm that was transparent so that the suspension of solids was easily visible. The bottom of the tank was elliptical in shape. The liquid depth was equal to the tank diameter. Two types of impellers were employed viz., six-bladed Rushton turbine of diameter 100 mm and four-bladed 45° pitched blade turbine of diameter 125 mm. The impeller off-bottom clearance is 62.5 mm. The vessel was fitted with four vertical baffles with a width of 25 mm and its height was equal to the height of liquid level in the contactor. The dimensions of the impellers chosen for this work are based on the observation of Chapman et al. (1983) and Pantula and Ahmed (1998) that the performance in terms of suspension quality at higher gas rates are much improved if larger diameter is employed. Similarly low clearance has been shown to enhance particle suspension capability (Nienow, 1968). For this experimental study, water ($\rho = 1000 \text{ kg/m}^3$) is used as the liquid phase, and ilmenite particles ($\rho = 4200 \text{ kg/m}^3$) in the size range of 120–250 μm is used as the solids phase. The gas phase considered was air and was introduced into the reactor by a pipe sparger with diameter of 10 mm, which is placed at a clearance of 25 mm from the center of the impeller. Fine stainless steel of wire mesh (0.2 mm opening) was wound around the outlet of the sparger. This was to prevent the suction of fines into the sparger. Agitation was carried out using a variable-speed DC motor and the speed of the agitation was noted using a tachometer. Power consumptions were computed using measured values of current and voltages. Other details of the present experiment study are available in the earlier published work (Geetha and Surender, 1997).
The experiments were carried out with different impeller types and different impeller speeds to determine the quality of solid suspension. The critical impeller speed of solid suspension were determined experimentally for four different solid loading rates, viz., 10, 20, 30 and 40 % by weight. The critical impeller speed for solid suspension is predicted by observing visually that the solids remain at the tank bottom for not more than 2 seconds (Zwietering, 1958). Since visual method is reported to be not very accurate for higher solid loading rates, an alternate method based on the measurement of variation in impeller power consumption with respect to the impeller speed was also used to determine the critical impeller speed. The same method was adapted by Rewatkar et al. (1991) for determination of $N_{J_s}$ and $N_{J_{sg}}$ for their reactors where the diameter of tank was ranging from 0.57 m to 1.5 m.
method, the graph of power number versus Reynolds number is plotted. Then the minimum value of the curve is taken as the critical impeller speed. This is shown in Figure 6.2.

![Graph of power number versus Reynolds number](image)

**Figure 6.2.** Prediction of critical impeller speed from the graphical plot of $N_{Re}$ vs. $N_p$ and the value obtained for critical impeller speed by visual method, is also shown in Table 6.2. The error percentage was calculated as

$$\text{Error} \% = \left( \frac{\text{CIS}_{\text{visual}} - \text{CIS}_{\text{graphical}}}{\text{CIS}_{\text{visual}}} \right) \times 100$$

It can be observed that the percentage of error is in the range of 3–6% for various operating conditions. Since the deviation is not much between both the approaches and visual method is much easier, this method is used for the determination of critical impeller speed for further experimental conditions.
Table 6.2. Values of critical impeller speed

<table>
<thead>
<tr>
<th>Particle size (μm)</th>
<th>Air flow rate (vvm)</th>
<th>Critical impeller speed, RPM</th>
<th>% of Error</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
<td>Visual method</td>
<td>Graphical method</td>
</tr>
<tr>
<td>230</td>
<td>0.5</td>
<td>330</td>
<td>315</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>428</td>
<td>415</td>
</tr>
<tr>
<td></td>
<td></td>
<td>529</td>
<td>559</td>
</tr>
</tbody>
</table>

6.3. CFD Modeling

6.3.1. Model Equations

The gas–liquid–solid flows in mechanically agitated contactor are simulated using Eulerian multi-fluid approach. Each phase is treated as different continua that interact with other phases everywhere in the computational domain. The motion of each phase is governed by respective Reynolds averaged mass and momentum conservation equations. The governing equations for each phase are given below:

**Continuity equation:**

\[
\frac{\partial}{\partial t} (\varepsilon_k \rho_k) + \nabla \cdot (\rho_k \varepsilon_k \bar{u}_k) = 0 \tag{6.1}
\]

where \( \rho_k \) is the density and \( \varepsilon_k \) is the volume fraction of phase \( k = g \text{ (gas)}, s \text{ (solid)}, l \text{ (liquid)} \) and the volume fraction of the three phases satisfy the following condition:

\[
\varepsilon_l + \varepsilon_g + \varepsilon_s = 1 \tag{6.2}
\]
**CFD Simulation of Gas-Liquid-Solid Mechanically Agitated Contactor**

**Momentum equations:**

Gas phase (dispersed fluid phase)

\[
\frac{\partial}{\partial t}(\rho_g \cdot e_g \cdot \bar{u}_g) + \nabla \cdot (\rho_g \cdot e_g \cdot \bar{u}_g \bar{u}_g) = -e_g \cdot \nabla P + \nabla \cdot \left( e_g \cdot \mu_{eff} \left[ \nabla \bar{u}_g + \left( \nabla \bar{u}_g \right)^T \right] \right) + \rho_g \cdot e_g \cdot \bar{g} - \bar{F}_{D_{lgs}}
\]

………………..(6.3)

Liquid phase (continuous phase)

\[
\frac{\partial}{\partial t}(\rho_l \cdot e_l \cdot \bar{u}_l) + \nabla \cdot (\rho_l \cdot e_l \cdot \bar{u}_l \bar{u}_l) = -e_l \cdot \nabla P + \nabla \cdot \left( e_l \cdot \mu_{eff} \left[ \nabla \bar{u}_l + \left( \nabla \bar{u}_l \right)^T \right] \right) + \rho_l \cdot e_l \cdot \bar{g} + \bar{F}_{D_{lgs}} + \bar{F}_{D_{lhn}} + \bar{F}_{TD}
\]

……………….. (6.4)

Solid phase (dispersed solid phase)

\[
\frac{\partial}{\partial t}(\rho_s \cdot e_s \cdot \bar{u}_s) + \nabla \cdot (\rho_s \cdot e_s \cdot \bar{u}_s \bar{u}_s) = -e_s \cdot \nabla P - \nabla P_s + \nabla \cdot \left( e_s \cdot \mu_{eff} \left[ \nabla \bar{u}_s + \left( \nabla \bar{u}_s \right)^T \right] \right) + \rho_s \cdot e_s \cdot \bar{g} - \bar{F}_{D_{lhs}} - \bar{F}_{TD}
\]

………………..(6.5)

where P is the pressure, which is shared by all the three phases, \( \mu_{eff} \) is the effective viscosity. The second term on the RHS of solid phase momentum equation (6.5) accounts for additional solids pressure which arise due to solids collision and the last term \( (F_D) \) in all the momentum equations (6.3)–(6.5) represent the drag force that arise due to the momentum exchange mechanism between the different phases.

**6.3.2. Interphase momentum transfer**

There are various interaction forces such as the drag force, the lift force and the added mass force etc. during the momentum exchange between the different phases. But the main interaction force is due to the drag force caused by the slip between the different phases. Recently, Khopkar et al. (2003, 2005) studied the influence of different interphase forces and reported that the effect of the virtual mass force is not significant in the bulk region of agitated reactors and the magnitude of the
Basset force is also much smaller than that of the inter-phase drag force. Further they also reported that the turbulent dispersion terms are significant only in the impeller discharge stream. Very little influence of the virtual mass and lift force on the simulated solid holdup profiles was also reported by Ljungqvist and Rasmuson (2001). Hence based on their recommendations and also to reduce the computational time, only the interphase drag force is considered in this work. In our CFD simulation, both the gas and the solid phases are treated as dispersed phases and the liquid phase is treated as continuous. Hence the drag force exerted by the dispersed phase on the continuous phase is calculated as follows:

The drag force between the liquid and solid phases is represented by the equation

$$\vec{F}_{D,ls} = C_{D,ls} \frac{3}{4} \rho_l d_p \|\vec{u}_l - \vec{u}_s\| (\vec{u}_s - \vec{u}_l)$$  \hspace{1cm} \text{.................(6.6)}$$

where the drag coefficient proposed by Brucato et al. (1998) is used.

$$\frac{C_{D,ls} - C_{D0}}{C_{D0}} = 8.67 \times 10^{-4} \left( \frac{d_p}{\lambda} \right)^3$$  \hspace{1cm} \text{.................(6.7)}$$

where, $d_p$ is the particle size and $\lambda$ is the Kolmogorov length scale, $C_{D0}$ is the drag coefficient in stagnant liquid which is given as

$$C_{D0} = \frac{24}{\text{Re}_p} \left( 1 + 0.15 \text{Re}_p^{0.687} \right)$$  \hspace{1cm} \text{.................(6.8)}$$

where $\text{Re}_p$ is the particle Reynolds number.

The drag force between the gas and liquid phases is represented by the equation

$$\vec{F}_{D,lg} = C_{D,lg} \frac{3}{4} \rho_l d_b \|\vec{u}_g - \vec{u}_l\| (\vec{u}_g - \vec{u}_l)$$  \hspace{1cm} \text{.................(6.9)}$$
where the drag coefficient exerted by the dispersed gas phase on the liquid phase is obtained by the modified Brucato drag model (Khopkar et al., 2003), which accounts for interphase drag by microscale turbulence and is given by

\[
\frac{C_{\text{D,lg}} - C_{\text{D}}}{C_{\text{D}}} = 6.5 \times 10^{-6} \left( \frac{d_p}{\lambda} \right)^3
\]  

where \( C_{\text{D}} \) is the drag coefficient of single bubble in a stagnant liquid and is given by

\[
C_{\text{D}} = \text{Max} \left( \frac{24}{Re_b} \left( 1 + 0.15Re_b^{0.687} \right) \frac{8Eo}{3Eo + 4} \right)
\]  

where \( Eo \) is Eotvos number, \( Re_b \) is the bubble Reynolds number and they are given by

\[
Re_b = \frac{\left| \bar{u}_l - \bar{u}_g \right| d_b}{\nu_l}
\]  

\[
Eo = \frac{g \left( \rho_l - \rho_g \right) d_b^2}{\sigma}
\]  

The only other non drag force considered in the present work is of turbulent dispersion. This turbulent dispersion force is the result of the turbulent fluctuations of liquid velocity which approximates a diffusion of the dispersed phase from higher region to lower region. The importance of modeling of turbulent dispersion in liquid–solid stirred tank is also highlighted in the literature (Ljungqvist and Rasmuson, 2001; Barrue et al., 2001). The following equation for the turbulent dispersion force derived by Lopez de Bertodano (1992) is used for the present simulation and is given by

\[
\bar{F}_{\text{TD}} = -C_{\text{TD}} \rho_l k_1 \nabla \bar{e}_l
\]  

where \( C_{\text{TD}} \) is a turbulent dispersion coefficient, and is taken as 0.1 for the present investigation.
In the present study, the standard $k-\varepsilon$ turbulence model for single phase flows has been extended for turbulence modeling of three phase flows in stirred reactors. The corresponding values of $k$ and $\varepsilon$ are obtained by solving the following transport equations for the turbulence kinetic energy and turbulence dissipation rate:

$$\frac{\partial (\varepsilon_i \rho_i k_i)}{\partial t} + \nabla \left( \varepsilon_i \rho_i \bar{u}_i k_i - \left( \mu + \frac{\mu_l}{\sigma_k} \right) \Delta k_i \right) = \varepsilon_i \left( P_i - \rho_i \varepsilon_i \right)$$

$$\text{...............}(6.15)$$

$$\frac{\partial (\varepsilon_i \rho_i \varepsilon_i)}{\partial t} + \nabla \left( \varepsilon_i \rho_i \bar{u}_i \varepsilon_i - \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \Delta \varepsilon_i \right) = \varepsilon_i \frac{\varepsilon_i}{k_i} \left( C_{e2} P_i - C_{e1} \rho_i \varepsilon_i \right)$$

$$\text{...............}(6.16)$$

where $C_{e1}=1.44$, $C_{e2}=1.92$, $\sigma_k=1.0$, $\sigma_\varepsilon=1.3$ and $P_i$, the turbulence production due to viscous and buoyancy forces, is given by

$$P_i = \mu_l \nabla \bar{u}_i \left( \nabla \bar{u}_i + \nabla \bar{u}_i^T \right) - \frac{2}{3} \nabla \bar{u}_i \left( 3 \mu_l \nabla \bar{u}_i + \rho_i k_i \right)$$

$$\text{...............}(6.17)$$

For the continuous phase (liquid phase) the effective viscosity is calculated as

$$\mu_{\text{eff},i} = \mu_l + \mu_{T,i} + \mu_{\text{tg}} + \mu_{\text{ts}}$$

$$\text{...............}(6.18)$$

where $\mu_l$ is the liquid viscosity, $\mu_{T,i}$ is the liquid phase turbulence viscosity or shear induced eddy viscosity, which is calculated based on the $k-\varepsilon$ model as

$$\mu_{T,i} = C_p \rho_{i} \frac{k_i^2}{\varepsilon_i}$$

$$\text{...............}(6.19)$$

$\mu_{\text{tg}}$ and $\mu_{\text{ts}}$ represent the gas and solid phase induced turbulence viscosity respectively and are given by

$$\mu_{\text{tg}} = C_{p_g} \rho_{1} \varepsilon_g \left| \bar{u}_g - \bar{u}_i \right|$$

$$\text{...............}(6.20)$$

$$\mu_{\text{ts}} = C_{p_s} \rho_{1} \varepsilon_s \left| \bar{u}_s - \bar{u}_i \right|$$

$$\text{...............}(6.21)$$

where $C_{p_{lg}}$ has a value of 0.6.
For gas and solid phases the respective effective viscosities are calculated as

\[ \mu_{\text{eff}, g} = \mu_g + \mu_{T, g} \]  
\[ \mu_{\text{eff}, s} = \mu_s + \mu_{T, s} \]

where \( \mu_{T, g} \) and \( \mu_{T, s} \) are the turbulence viscosity of gas and solid phases respectively.

The turbulent viscosity of the gas phase and the solids phase is related to the turbulence viscosity of the liquid phase and are given by equations (6.24) and (6.25) (Jakobsen et al., 1997)

\[ \mu_{T, g} = \frac{\rho_g}{\rho_l} \mu_{T, l} \]  
\[ \mu_{T, s} = \frac{\rho_s}{\rho_l} \mu_{T, l} \]

6.3.4. Closure law for solids pressure

The solids phase pressure gradient results from normal stresses resulting from particle–particle interactions, which become very important when the solid phase fraction approaches the maximum packing. This solid pressure term is defined based on the concept of elasticity, which is described as a function of elasticity modulus and solid volume fraction. The most popular constitutive equation for solids pressure as given by Gidaspow (1994) is

\[ \nabla P_s = G(\varepsilon_s) \nabla \varepsilon_s \]

where \( G(\varepsilon_s) \) is the elasticity modulus and it is given as

\[ G(\varepsilon_s) = G_0 \exp(c(\varepsilon_s - \varepsilon_{sm})) \]

as proposed by Bouillard et al. (1989), where \( G_0 \) is the reference elasticity modulus, \( c \) is the compaction modulus and \( \varepsilon_{sm} \) is the maximum packing parameter.
### 6.4. Numerical Methodology

In this work, the commercial CFD software ANSYS CFX-10 is used for the steady state hydrodynamic simulation of gas–liquid–solid flows in the mechanically agitated contactor. The details of the reactor geometry used for CFD simulation and the operating parameters are given in Table 6.3. Steady state simulations are performed for different types of impellers, agitation speeds, particle diameter, solid concentration, and superficial gas velocity. Due to the symmetry of geometry, only one-half of the agitated contactor is considered as the computational domain and is discretised using block structured grids, which allows finer grids in regions where higher spatial resolutions are required. The blocks are further divided into finer grids.
**CFD Simulation of Gas-Liquid-Solid Mechanically Agitated Contactor**

Around 200,000 total computational nodes are created using the structured hexa mesh option of ICEM CFD in order to get the grid independent solution for the flow. Figure 6.3 depicts a typical mesh used for the numerical simulation in this work.

During the last few decades, various approaches have been proposed in the literature for the simulation of impeller rotation. The most widely used approach in the literature is the multiple frame of reference (MFR) approach, in which the tank is divided into two regions: a rotating frame that encompasses the impeller and the flow surrounding it and a stationary frame that includes the tank, baffles, and the flow outside the impeller frame. The boundary between the inner and outer region have to be selected in such a way that the predicted results are not sensitive to its actual location. The other approach is the sliding grid approach, in which the inner region is rotated during computation and slide along the interface with the outer region. This method is fully transient and is considered as more accurate, but it requires more computational time when compared to MFR. Hence in this work, the MFR approach is used for simulating the impeller rotation. In the MFR approach, the computational domain is divided into an impeller zone (rotating reference frame) and a stationary zone (stationary reference frame). The interaction of inner and outer regions is accounted for by a suitable coupling at the interface between the two regions where the continuity of the absolute velocity is implemented. The boundary between inner and outer region is located at \( r/R = 0.6 \). No-slip boundary conditions are applied on the tank walls and shaft. The free surface of tank is considered as the degassing boundary condition. Initially the solid particles are distributed in a homogeneous way inside the whole computational domain.
The bubble size distribution in the mechanically agitated reactor depends on the design and operating parameters and there is no experimental data available for bubble size distribution. It has been reported by Barigou and Greaves (1992) that their bubble size distribution is in the range of 3.5–4.5 mm for the higher gas flow rates used in their experiments. Also in the recent simulation study on a gas–liquid stirred tank reactor carried out by Khopkar et al. (2005) a single bubble size of 4 mm was assumed. Since the gas flow rates used in our experiments are also in the same range, a mean bubble size of 4 mm is assumed for all our simulations. Further, the validity of bubble size used in the CFD simulation is rechecked by calculating the bubble size based on the reported correlations in literature (Calderbank and Moo-Young, 1961) using the simulation results of gas holdup and power consumption values. The mean bubble size is calculated according to the following correlation as

\[ d_b = 4.15 \left( \frac{\rho \varepsilon^{0.4}}{\sigma^{0.6}} \right)^{-1} e^{0.5} + 0.0009 \] .................(6.28)

The value obtained for mean bubble size is around 3.7 mm. Hence for further simulations, the bubble size of 4 mm is used.

The discrete algebraic governing equations are obtained by element-based finite volume method. The second-order equivalent to high-resolution discretisation scheme is applied for obtaining algebraic equations for momentum, volume fraction of individual phases, turbulent kinetic energy, and turbulence dissipation rate. Pressure–velocity coupling was achieved by the Rhie-Chow algorithm (1994). The governing equations are solved using the advanced coupled multigrid solver technology of ANSYS CFX-10. The criteria for convergence is set as \(1 \times 10^{-4}\) for the rms (root mean square) residual error for all the governing equations. The rms
residual is obtained by taking all of the residuals throughout the domain, squaring them, taking the mean, and then taking the square root of the mean for each equation. The simulations are carried out on the eight nodes, 32 processor AMD64 cluster with a clock speed of 2.55 GH and 8 GB memory for each node.

![Computational grid of mechanically agitated three-phase contactor](image)

**Figure 6.3.** Computational grid of mechanically agitated three-phase contactor used in the present study (a) Tank (b) DT (c) PBTD

### 6.5. Results and Discussion

#### 6.5.1. Solid–liquid flows in an agitated contactor

Since any CFD model has to be validated first, we have carried out CFD simulations of gas–liquid and solid–liquid flows in mechanically agitated contactor. The experimental results taken for validation of the CFD model are

(a) The experimental data obtained by computer automated radioactive particle tracking (CARPT) technique by Guha et al. (2007) for the case of liquid–solid agitated contactor with a radial type impeller (DT)

(b) The experimental data obtained by Spidla et al. (2005) using a conductivity probe for a pilot plant stirred vessel of 1m in diameter which is stirred with 6-pitched blade turbine (axial type impeller)
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For the case of DT, Guha et al. (2007) characterised the solid hydrodynamics in a solid–liquid stirred tank reactor using computer automated radioactive particle tracking (CARPT) and measured axial and radial distribution of solid axial velocity for overall solid holdup of 7% at impeller speed of 1200 rpm. The variation of non-dimensional solid velocity components of axial, radial & tangential \( (U/U_{\text{tip}}, \pi D N) \) along the non-dimensional axial directions \( (z/T) \) are plotted in Figure 6.4 (a-c) for the case of DT at a radial position of \( r/R = 0.5 \). The experimental data plotted in Figure 6.4(a-c) corresponds to the data given by Guha et al. (2007). It can be observed that the axial variation of the axial component of solid velocity agrees well with the experimental results.

![Axial profiles of radial component of solid velocity](image)

**Figure 6.4 (a).** Axial profiles of radial component of solid velocity
Figure 6.4 (b). Axial profile of the tangential component of the solids velocity

Figure 6.4(c). Axial profiles of the axial component of solid velocity
But for the other two components, eventhough there is a quantitative agreement between experimental and simulation results, there is a discrepancy between numerical simulations and experimental results qualitatively near the impeller region. This may be due to the fact that the mean velocity components of fluid mainly depend on the turbulent fluctuations and these turbulent fluctuations dominate mainly at the impeller region of stirred tank and the turbulence model used in the present study is not able to capture properly the strong turbulence near the impeller region.

Similarly non-dimensional radial profiles \( ((r-R_i)/(R-R_i)) \), where \( R_i \) is the impeller radius) of various components of non-dimensional solid velocity at the axial position of \( z/T= 0.34 \) is shown in Figure 6.5 (a-c).

![Figure 6.5 (a). Radial profiles of the radial component of the solids velocity](image)
Figure 6.5 (b). Radial profiles of the tangential component of the solids velocity

Figure 6.5 (c). Radial profiles of the axial component of the solids velocity
The same trend is observed in this case also. This type of discrepancy is confirmed by Guha et al. (2008) where they have carried out Large Eddy Simulation and Euler–Euler simulation of solid suspension in stirred tank reactor and concluded that there are major discrepancies in the prediction of solid velocities by both the numerical methods near the impeller region.

Similarly for the case of axial type impeller, experimental data of Spidla et al. (2005) have been used for the comparison of the axial solid distributions. They have presented detailed particle distribution data using a conductivity probe for a pilot plant stirred vessel of 1 m in diameter which is stirred with a six pitched blade turbine (PBTD). Figure 6.6 shows the comparison between the CFD simulation results and the experimental results for axial distribution of solid volume fraction at the radial position of $r/R = 0.8$ for an overall solid holdup of 10% at the critical impeller speed of 267 rpm for the case of PBTD impeller. A good comparison exists between CFD prediction and experimental results for axial solid concentration.

![Axial solid concentration profile for PBTD in solid-liquid stirred reactor (solids loading = 10%, impeller speed = 267 rpm, $r/R = 0.8$)](image)

**Figure 6.6.** Axial solid concentration profile for PBTD in solid-liquid stirred reactor (solids loading = 10%, impeller speed = 267 rpm, $r/R = 0.8$)
For the case of gas–liquid flows in an agitated contactor, CFD model predictions of radial profiles of liquid velocity are validated with the experimental data of Aubin et al. (2004) for the pitched blade turbine with downward (PBTD) and upward (PBTU) pumping. They have used particle image velocimetry to investigate the liquid phase hydrodynamics. For the case of PBTD, the radial profile of the axial component of liquid velocity is shown in Figure 6.7 at the axial position $z/T = 0.31$. The impeller speed is taken as 300 rpm. Similar results are shown in Figure 6.8 for the case of PBTU with the same impeller speed. It can be seen clearly from both the figures that there exists excellent agreement between the CFD simulations and experimental data.

![Figure 6.7](image)

**Figure 6.7.** Radial profiles of dimensionless axial liquid velocity at various axial locations for the case of PBTD (impeller speed = 300 rpm, $z/T = 0.31$)
6.5.2.1. Gross flow field characteristics

The gross flow field characteristics of mechanically agitated reactor are generally characterised by power number, pumping number and pumping efficiency. Since the overall prediction of CFD is good, CFD simulation is used further to calculate these values. The pumping number \( N_Q \) and power number \( N_p \) are calculated as follows:

\[
N_Q = \frac{2 \int_0^r \pi r U dr}{\pi D^3} \tag{6.29}
\]

The limits of integration for the radial distance are from the surface of the shaft to the impeller radius and \( U \) is the axial liquid velocity.

\[
N_p = \frac{P}{\rho N^3 D^5} \tag{6.30}
\]
The pumping efficiency is then calculated by the following equation

\[
Pumping \text{ efficiency} = \frac{N_Q}{N_P} \quad \ldots (6.31)
\]

The Power draw (P) is determined from torque equation (\( P = 2\pi NT \)) and the total torque can be calculated from the torque acting on all the blades.

The predicted values of pumping number and power number are compared with experimental data and are shown in Table 6.4. It can be observed that the values predicted by CFD simulations agree reasonably well with the experimental values but the overall gas holdup predicted by CFD simulation is slightly varies with the experimental values. This may be because the gas holdup mainly depends on the bubble size distribution, which is not included in the present study.

**Table 6.4.** Gross Characteristics of Gas–liquid Stirred Vessel

<table>
<thead>
<tr>
<th>Operating condition</th>
<th>Total gas holdup</th>
<th>Power number (Np)</th>
<th>Pumping number (NQ)</th>
<th>Pumping efficiency (NQ/Np)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental (Aubin et al., 2004)</td>
<td>CFD</td>
<td>Experimental (Aubin et al., 2004)</td>
<td>CFD</td>
<td>Experimental (Sardeing et al., 2004)</td>
</tr>
<tr>
<td>PBTU N =300 RPM</td>
<td>0.037</td>
<td>0.042</td>
<td>1.56</td>
<td>1.3</td>
</tr>
<tr>
<td>PBTU N =300 RPM</td>
<td>0.058</td>
<td>0.052</td>
<td>1.80</td>
<td>1.5</td>
</tr>
</tbody>
</table>

**6.5.3. Gas–liquid–solid flows in an agitated contactor**

In this section, CFD simulation has been used for simulating the hydrodynamics of gas–liquid–solid flows in an agitated contactor. Recently Murthy et al. (2007) have carried out detailed investigations on gas–liquid–solid stirred reactor
using CFD simulation for the case of lower solids concentration (2–15 wt.%) and for low-density particles. Their results clearly highlight the capability of CFD in predicting the gross characteristics of such three-phase systems. Also, only the standard deviation approach was used by these authors to characterise the critical impeller speed. In this work, we have carried out CFD simulation for the gas–liquid–solid mechanically agitated contactor with high density ilmenite particles as solids phase and with solid loading in the range of (10–30 wt.%).

Further, for the case of three-phase systems, experimental data for gas and solid holdup profile are very limited or not available. Therefore, the present simulations have been focused on the prediction of the critical impeller speed for gas–liquid–solid mechanically agitated contactor for different type of impellers, for various gas flow rates and different particle sizes. The critical impeller speed is determined from CFD simulation using both the standard deviation approach and cloud height criteria. The values obtained by CFD simulation for critical impeller speed is compared with our experimental data. Also the qualitative features of the flow pattern predicted by CFD simulation are presented in the following sections.

6.5.3.1. Flow field

The geometry chosen for this simulation is the reactor shown in Figure 6.1. The reactor dimensions and the physical properties of all the phases considered are given in Table 6.3.
The liquid phase chosen is water and the solid phase considered for the present study corresponds to high density ilmenite particles ($\rho_s = 4200 \text{ kg/m}^3$) with particle size 230 $\mu\text{m}$ and with 30% solids loading by weight. The gas phase is air and the flow rate is taken as 0.5 vvm. Two types of impellers are considered for the simulation. One is axial type impeller (PBTD) and the other is radial type impeller (DT). Figures 6.9 (a & b) shows the solid velocity profile obtained for the two types of impellers where the impeller speed chosen for both the cases correspond to that of critical impeller speed. As can be seen clearly from Figure 6.9 (a) that, for the case of DT, there exists circular loops of solids above and below the impeller and there is a radial jet flow of solids flow in the impeller stream. For the case of PBTD impeller (Figure 6.9(b)), there is only one circulation loop for solids, where the solids move upward towards the surface of liquid and then turn downwards to the bottom. The flow field
The turbulence kinetic energy predicted by CFD simulation at the midbaffle plane for the case of DT and PBTD impellers shown in Figure 6.10. It can be clearly seen from Figures 6.10 (a & b) that DT impeller generates high intensity turbulence near the tip of the impeller blade which gets dissipated very quickly, whereas the PBTD impeller generates the medium intensity turbulence, which gives better distribution of turbulence over the entire vessel of stirred tank.

![Turbulence kinetic energy profile predicted by CFD simulation in gas–liquid–solid stirred reactor for the case of (a) DT (b) PBTD (gas flow rate = 0.5 vvm, particle size = 230 μm & particle loading =30 wt %)](image)

Since the energy dissipation rate plays an important role in solids suspension in agitated reactors, the energy dissipation rate obtained by CFD simulation for both DT and PBTD impellers with respect to the gas flow rate is shown in Table 6.5. The values presented in the table are generated at the critical impeller speed with a solid loading of 30% by weight. It can be observed from the results that the energy
dissipation rate is higher for the case of DT. It can also be seen from the table that under ungassed conditions (solid–liquid agitated reactors) the energy dissipation rate for DT impellers is approximately 1.5 times the energy dissipation rate for PBTD impellers. For the case of gas–liquid–solid agitated contactors, the energy dissipation rate increases with increase in gas flow rates. This increase in energy dissipation rate is slightly more for PBTD impellers (2 times) than for DT impellers (1.7 times). This may be due to instabilities due to large fluctuations in impeller power at the higher gas flow rate for PBTD and this observation is in agreement with those reported in literature (Nienow et al., 1985; Bujalski et al., 1988).

Table 6.5. Energy dissipation rate obtained by CFD simulation for different type of impellers (particle size = 230 μm & particle loading = 30 wt. %)

<table>
<thead>
<tr>
<th>Air flow rate (vvm)</th>
<th>Energy dissipation rate, m²/s³</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>DT</td>
</tr>
<tr>
<td>0</td>
<td>0.66</td>
</tr>
<tr>
<td>0.5</td>
<td>0.97</td>
</tr>
<tr>
<td>1.0</td>
<td>1.65</td>
</tr>
</tbody>
</table>

6.5.3.2. Liquid phase mixing

Generally the mixing performance is of crucial importance in turbulent mechanically agitated reactors. A global characterisation of such passive scalar mixing is the mixing time. Roughly speaking, it is the time to achieve complete (that is, over the whole vessel) homogenisation of an added passive scalar. It is generally defined as the time required to mix the added passive tracer with the contents of the tank until a certain degree of uniformity is achieved. But, usually the precise
definition of a certain degree of uniformity gives rise to little confusion. The definition of what is considered homogeneous varies from study to study. The degree of homogeneity considered in the present study is 95% which means that the concentration variations are smaller than 5% of the fully mixed concentration. The convection–diffusion equation for species transport equations for tracer addition to the stirred tank are solved till degree of mixing is achieved. The mixing time obtained from the CFD simulation are analysed based on a simplified model proposed by Kawase and Moo-Young (1989). They developed a correlation for mixing time in single-phase stirred tank reactors on the basis of Kolmogorov’s theory of isotropic turbulence. Their correlation for single phase system is a function of energy dissipation and is given as

\[ \theta_m = 6.35 \times 2^{\frac{(5n-2)n}{3}} D_T^{2/3} \varepsilon^{-1/3} = 12.7 D_T^{2/3} \varepsilon^{-1/3} \]

In the above equation \( D_T \) is the diameter of the tank and \( \varepsilon \) is the energy dissipation rate and \( n \) is the flow index of the power law model. In this work, the extent of above correlation is examined for two- and three-phase systems by using the energy dissipation rate for the systems obtained from CFD simulation. Similar type of comparisons have also been reported in the literature (Kawase and Shimizu, 1997; Dohi et al., 1999). Figure 6.11 shows the comparison of liquid-phase mixing time for three-phase systems with the correlation given by equation (6.32) for both radial type (DT) and axial type impellers (PBTD). The deviation of the predicted values of mixing time by simulation from that of equation (6.32) is around 5% for DT and around 8 % for PBTD. It can also be seen from this figure that the value of mixing time decreases with an increase in impeller speed. This is due to the fact that eventhough, the suspension quality increases with an increase in impeller speed, more
amount of energy is spent at the solid–liquid interface and hence only less energy is available for liquid-phase mixing.

![Graph showing mixing time variation with impeller speed](image)

**Figure 6.11.** Mixing time variation with impeller speed

### 6.5.3.3. Solid suspension studies

CFD simulation of three-phase mechanically agitated contactor is undertaken in this study to verify quantitatively the solid suspension characteristics since the important consideration for design and operation of these types of reactors is the determination of the state of suspension. The quality of solid suspension is evaluated by the extent of off-bottom suspension i.e., critical impeller speed for just suspended state and extent of axial solid distribution i.e., solid suspension height. Generally Zwietering criteria (the impeller speed at which the particles do not remain stationary at the bottom of the vessel) is used for characterising the off-bottom suspension. But incorporating Zwietering criteria is difficult in the Eulerian–Eulerian approach of the present CFD simulation. Hence the method proposed by Bohnet and Niesmak (1980) which is based on the value of standard deviation is used in the present study for the
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prediction of critical impeller speed. This standard deviation method was also
successfully employed for liquid–solid suspension by various authors (Khopkar et al.,
2006; Murthy et al., 2007). It is defined as

\[ \sigma = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left( \frac{C_i}{C_{avg}} - 1 \right)^2} \] ..........................(6.33)

where \( n \) is the number of sampling locations used for measuring the solid holdup.

The increase in the degree of homogenisation (better suspension quality) is
manifested in the reduction of the value of standard deviation. The standard deviation
is broadly divided into three ranges based on the quality of suspension. For uniform
suspension the value of the standard deviation \( \sigma \) is found to be smaller than 0.2
(\( \sigma < 0.2 \)), for just suspended condition the value of the standard deviation is between
0.2 & 0.8 (0.2 < \( \sigma < 0.8 \)) and for an incomplete suspension the standard deviation value
is greater than 0.8 (\( \sigma > 0.8 \)). But it is very difficult to exactly find the critical impeller
speed required for the just suspended state from the values of the standard deviation.
These difficulties were also cited in the literature (Khopkar et al., 2006, van der
Westhuizen et al., 2008). Hence we have used another criteria which is based on the
solid suspension height i.e., cloud height (\( H_{cloud} = 0.9H \)) along with standard deviation
method. Kraume (1992) used these two criteria to evaluate the critical impeller speed
in liquid–solid suspension. For the present study, both these criteria have been used
to evaluate the quality of solid suspension and to determine the critical impeller speed.
Systematic investigation of solids suspension using CFD simulation has been carried
out for different processing and operating conditions. The critical impeller speed
obtained by CFD simulation based on these two criteria is validated with our
experimental data.
6.5.3.3.1. Effect of impeller type

CFD simulations have been carried out for 6 blade Rushton turbine impeller (DT) and 4 blade pitched blade turbine with downward pumping (PBTD) at different impeller speeds. The air flow rate for this simulation is 0.5 vvm and the solid phase consists of ilmenite particles of size 230 μm and the solid loading is 30% by weight.

![Variation of standard deviation values with respect to the impeller speed for DT and PBTD](image1)

**Figure 6.12.** Variation of standard deviation values with respect to the impeller speed for DT and PBTD

![CFD prediction of cloud height with respect to the impeller speed for DT](image2)

**Figure 6.13.** CFD prediction of cloud height with respect to the impeller speed for DT (gas flow rate = 0.5 vvm, particle size = 230 μm & particle loading = 30 wt.%)
Figure 6.14. CFD prediction of cloud height with respect to the impeller speed for PBTD (gas flow rate = 0.5 vvm, particle size = 230 μm & particle loading = 30 wt %)

Figure 6.12 shows the variation of the standard deviation value with respect to impeller speed for DT and PBTD. The value of standard deviation decreases with increase in impeller speed for both the impellers. Figure 6.13 depicts the predicted cloud height for the three impeller rotational speeds (7.83, 8.67, and 9.5 rps) for DT and Figure 6.14 shows the predicted cloud height for PBTD for three different impeller speeds (6.3, 7.13, and 7.97 rps).

It can be seen clearly from these figures that there is an increase in the cloud height with an increase in the impeller rotational speed. Similar observations were also reported by Khopkar et al. (2006). The values of standard deviation and cloud height obtained by CFD simulation along with experimental values for both the type of impellers are presented in Table 6.6. Based on these two criteria, it is found that the critical impeller speed required for DT is 8.67 rps and for PBTD is 7.13 rps which
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agrees very well with the experimental observation. It has to be noted again that both
the criteria have to be satisfied for critical impeller speed determination.

Table 6.6. Effect of impeller type on quality of suspension (gas flow rate = 0.5
vvm, particle size = 230 μm, & particle loading = 30 wt %)

<table>
<thead>
<tr>
<th>Type of impeller</th>
<th>Critical impeller speed, rps</th>
<th>Standard deviation, σ</th>
<th>Cloud height</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Experimental</td>
<td>CFD simulation</td>
<td></td>
</tr>
<tr>
<td>DT</td>
<td>8.67</td>
<td>8.67</td>
<td>0.66</td>
</tr>
<tr>
<td>PBTD</td>
<td>7.13</td>
<td>7.13</td>
<td>0.64</td>
</tr>
</tbody>
</table>

Figures 6.15(a & b) show dimensionless axial concentration profiles for the
DT and PBTD for various impeller speeds. The process conditions used are same as
before. It can be seen that the amount of solid particles that settles at the bottom of the
vessel decreases with increase in impeller rotational speed. The power required for
DT is two times more than that of PBTD for the same operating conditions. For
example, for solid loading of 30% wt, for the air flow rate of 0.5 vvm, DT requires
2.02 KW/m^3 of power while PBTD requires only 0.91 KW/m^3 of power. This lower
power requirement for PBTD impeller can be attributed to the fact that travel length
of fluid flow is lower for PBTD than for DT i.e., flow field generated by PBTD start
from the tip of the impeller region and is directed towards the tank bottom which is
responsible for solid suspension whereas liquid flow generated by DT travel in the
radial direction and splits into two streams, one above and one below the impeller and
only this lower stream of flow is associated with solid suspension. Hence DT requires
more power.
Figure 6.15. Axial concentration profiles predicted by CFD simulation for different impellers of (a) DT (b) PBTD (gas flow rate = 0.5 vvm, particle size = 230 μm & particle loading = 30 wt %)
It has been reported in the literature that the critical impeller speed depends on the particle size. Hence, CFD simulations have been carried out for three different particle sizes viz, 125 μm, 180 μm and 230 μm at the solid loading of 30 % by wt. and a gas flow rate of 0.5 vvm with both DT and PBTD type impellers. From the CFD simulation, the standard deviation and cloud height values are also obtained and they are shown in Table 6.7.

Table 6.7. Effect of particle size on quality of suspension (gas flow rate = 0.5 vvm & particle loading 30 = wt %)

<table>
<thead>
<tr>
<th>Particle diameter (μm)</th>
<th>DT</th>
<th></th>
<th></th>
<th>PBTD</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Critical impeller speed, rps</td>
<td>Standard deviation, σ</td>
<td>Cloud height</td>
<td>Critical impeller speed, rps</td>
<td>Standard deviation, σ</td>
</tr>
<tr>
<td></td>
<td>Experimental</td>
<td>CFD</td>
<td></td>
<td>Experimental</td>
<td>CFD</td>
</tr>
<tr>
<td>125</td>
<td>5.67</td>
<td>5.67</td>
<td>0.50</td>
<td>0.90</td>
<td>5.42</td>
</tr>
<tr>
<td>180</td>
<td>6.25</td>
<td>6.92</td>
<td>0.75</td>
<td>0.89</td>
<td>5.77</td>
</tr>
<tr>
<td>230</td>
<td>8.67</td>
<td>8.67</td>
<td>0.66</td>
<td>0.90</td>
<td>7.13</td>
</tr>
</tbody>
</table>

It can be seen clearly that critical impeller speed predicted by CFD simulation based on the criteria of standard deviation and solid cloud height agrees very well with the experimental data. Further, from Figure 6.16 it can be observed that the critical impeller speed for solid suspension increases with an increase in the particle size for fixed set of operating conditions and impeller configuration. This is due to the fact that with increase in the particle size, the terminal settling velocity increases. This settling velocity of particle causes sedimentation which in turn affects the solids
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suspension. Also it can be noted that an increase in particle size by two times results in an increase in critical impeller speed by approximately 1.5 times.

Figure 6.16. Effect of particle size on Critical impeller speed for different impellers (gas flow rate = 0.5 vvm & particle loading = 30 wt %)

6.5.3.3.3 Effect of air flow rate

CFD simulations have further been carried out to study the effect of air flow rate on the critical impeller speed for gas–liquid–solid mechanically agitated contactor. Figure 6.17 shows the comparison of CFD predictions with the experimental data on critical impeller speed for both the type of impellers at various gas flow rates (0 vvm, 0.5 vvm and 1.0 vvm). The values of the standard deviation and cloud height with respect to the impeller speed for different gas flow rates with different type of impellers are shown in Table 6.8.
Figure 6.17. Effect of air flow rate on Critical impeller speed for different impellers (particle size = 230 μm & particle loading = 30 wt %)

Table 6.8. Effect of air flow rate on quality of suspension for different type of impellers (particle size = 230 μm & particle loading = 30 wt. %)

<table>
<thead>
<tr>
<th>Air flow rate (vvm)</th>
<th>DT Experimental</th>
<th>CFD</th>
<th>Standard deviation, σ</th>
<th>Cloud height</th>
<th>PBTD Experimental</th>
<th>CFD</th>
<th>Standard deviation, σ</th>
<th>Cloud height</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>7.17</td>
<td>7.67</td>
<td>0.80</td>
<td>0.89</td>
<td>5.5</td>
<td>6.67</td>
<td>0.80</td>
<td>0.90</td>
</tr>
<tr>
<td>0.5</td>
<td>8.67</td>
<td>8.67</td>
<td>0.66</td>
<td>0.90</td>
<td>7.13</td>
<td>7.13</td>
<td>0.64</td>
<td>0.91</td>
</tr>
<tr>
<td>1.0</td>
<td>10.2</td>
<td>9.2</td>
<td>0.66</td>
<td>0.90</td>
<td>8.82</td>
<td>8.82</td>
<td>0.71</td>
<td>0.93</td>
</tr>
</tbody>
</table>
It can be observed that CFD simulation is capable of predicting the critical impeller speed in terms of standard deviation value and cloud height with an increase in gas flow rate for both types of impellers. Figure 6.18 shows solid volume fraction distribution predicted by CFD at the critical impeller speed for the solid loading of 30% by wt. and particle size of 230 μm with different air flow rates (0, 0.5, 1.0 vvm).

Figure 6.18. Effect of air flow rate on solid concentration distribution for DT by CFD simulations at the critical impeller speed (a) 0 vvm (b) 0.5 vvm (c) 1.0 vvm (particle size = 230 μm and particle loading = 30 wt. %)

Figure 6.19 shows the variation of standard deviation value with respect to the impeller speed. It can be seen that the reduction rate of standard deviation value in ungassed condition is more with increasing impeller speed when compared with gassed condition. Similarly for the case of higher gas flow rate, the reduction rate in the standard deviation value is much lower compared to lower gas flow rate. This is due to the presence of gas which reduces both turbulent dispersion and fluid circulation action of the impeller.
Since the quality of suspension is reduced due to decrease in impeller pumping capacity when gas is introduced in a suspended medium, there is a need to increase the impeller speed for re-suspension. This extent of increase in the impeller speed was found to depend upon gas flow rate \( (Q_g) \). In literature, various authors (Chapman et al., 1983; Nienow et al., 1985; Bujalski et al., 1988; Wong et al., 1987; Dutta and Pangarkar, 1995) have proposed a linear correlation between the difference in critical impeller speed for suspension with gas and without gas with the air flow rate as

\[
\Delta N_{js} = N_{js} - N_{jsg} = aQ_g 
\]

where \( a \) is a constant, \( N_{js} \) is the critical impeller speed without gas, while \( N_{jsg} \) is critical impeller speed under gas sparging conditions. Table 6.9 shows the value ‘\( a \)’ reported by various authors as well as by present CFD simulation. The operating conditions chosen for the present CFD simulation is solid particles of size 230 μm with solid loading of 30% by wt. and the impeller type chosen is DT.
It can be shown that there is a significant variation in the parameter value ‘a’ between different studies. This may be due to the variation in operating conditions such as particle size, loading and impeller diameter. It varies from 0.94 to 3.75. The values obtained from Nienow et al. (1985) and Bujalski et al. (1988) show the smallest dependence of critical impeller speed on air flow rate while those by Dutta and Pangarkar (1995) and Chapman et al. (1983) show the largest dependence. The value predicted by CFD simulation is around 1.53.

The extent of increase in critical impeller speed with increasing air flow rate is also different for different type of impellers. The increase in $N_{jsg}$ for PBTD is higher than DT. When gas flow increases from 0.5 vvm to 1.0 vvm, DT requires the lowest $N_{jsg}$ which is approximately 5.7% more, whereas PBTD requires 19% times more in the increase in the $N_{jsg}$. This may be due to the instabilities due to the large fluctuations in impeller power at the higher gas flow rate for PBTD and also due to the flow generated by the PBTD impeller is directly opposite to the flow of gas. This observation is in agreement with those reported in literature (Chapman et al., 1983; Bujalski et al., 1988).

<table>
<thead>
<tr>
<th>Reference</th>
<th>Value of the parameter ‘a’ in equation (6.34)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chapman et al.(1983) and Nienow et al.(1985)</td>
<td>0.94</td>
</tr>
<tr>
<td>Bujalski et al.(1988)</td>
<td>0.65</td>
</tr>
<tr>
<td>Wong et al.(1987)</td>
<td>2.03</td>
</tr>
<tr>
<td>Dutta and Pangarkar (1995)</td>
<td>3.75</td>
</tr>
<tr>
<td>Present CFD simulation</td>
<td>1.53</td>
</tr>
</tbody>
</table>
6.6. Conclusions

1. In this present work, Eulerian multi-fluid approach along with standard k-ε turbulence model has been used to study the solid suspension in gas–liquid–solid mechanically agitated contactor.

2. The results obtained from CFD simulations are validated qualitatively with literature experimental data (Guha et al., 2007; Spidla et al., 2005; Aubin et al., 2004) in terms of axial profiles of solid velocity in liquid–solid stirred suspension and liquid velocity in gas–liquid stirred suspension for different operating conditions. A good agreement was found between the CFD prediction and experimental data.

3. For gas–liquid–solid flows, the CFD predictions are compared quantitatively with our experimental data in terms of critical impeller speed based on the criteria of standard deviation method and cloud height in a mechanically agitated contactor. An adequate agreement was found between CFD prediction and experimental data.

4. The numerical simulation has further been extended to study the effect of impeller design (DT, PBTD), impeller speed, particle size (125–230 μm) and air flow rate (0–1.0 vvm) on the prediction of critical impeller speed for solid suspension in gas–liquid–solid mechanically agitated contactor.