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CFD SIMULATION OF SOLIDS SUSPENSION IN STIRRED TANKS: REVIEW

Many chemical reactions are carried out using stirred tanks, and the efficiency of such systems depends on the quality of mixing, which has been a subject of research for many years. For solid–liquid mixing, traditionally the research efforts were geared towards determining mixing features such as off-bottom solid suspension using experimental techniques. In a few studies that focused on the determination of solids concentration distribution, some methods that have been used have not been accurate enough to account for some small scale flow mal-distribution such as the existence of dead zones. The present review shows that computational fluid dynamic (CFD) techniques can be used to simulate mixing features such as solids off-bottom suspension, solids concentration and particle size distribution and cloud height. Information on the effects of particle size and particle size distribution on the solids concentration distribution is still scarce. Advancement of the CFD modeling is towards coupling the physical and kinetic data to capture mixing and reaction at meso- and micro-scales. Solids residence time distribution is important for the design, however, the current CFD models do not predict this parameter. Some advances have been made in recent years to apply CFD simulation to systems that involve fermentation and anaerobic processes. In these systems, complex interaction between the biochemical process and the hydrodynamics is still not well understood. This is one of the areas that still need more attention.

Stirred tanks have applications in many chemical processes where mixing is important for the overall performance of the system. In such systems, detailed information on the fluid characteristics resulting from the effect of the tank and impeller geometries is required [1,2]. Computational fluid dynamics (CFD) techniques have been used in the recent years to provide such information on the flow field [3,4]. This information is required for the determination of the hydrodynamic and design parameters. Hydrodynamics and mixing efficiency in stirred tanks are important for the design of many industrial processes such as precipitation, flotation and biochemical processes. In such systems, mass transfer processes limit the overall rate of reaction, and is driven by the impeller generated convective motion at larger scales, by turbulent transfer at smaller scales and down to diffusion at molecular scales [5].

Recently, some efforts have been made to apply CFD simulation techniques to model biological systems like anaerobic digesters [6,7] and fermenters [8]. These systems involve complex interactions of shear, mass transfer and reaction kinetics. Simulation of such systems, especially at large a scale, requires very intensive computational work. However, a large body of work is still found in the areas of hydrodynamics and mixing.

The objective of this work is to give a summary of the work on the CFD simulation of solid–liquid mixing in stirred tanks and to analyze the research trends in this field. The focus is on the hydrodynamic aspect such as cloud height, off-bottom solids suspension, cloud height and drag/non-drag forces.

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Hydrodynamics

In multiphase reaction processes, hydrodynamic characteristics influence phase mixing and mass transfer, and these affect conversion in the reactor. The relative influence of the hydrodynamic parameters on the mixing performance of a stirred tank may vary with the detailed system specifications, which keep changing with time.

In solid–liquid systems, it is important to determine the distribution of the solids in the tank in accordance with the process requirements. Some processes require that the particles are just suspended off the bottom, whilst, in some processes, complete off-bottom solids suspension is necessary. After the complete off-bottom solid suspension, the solids concentration distribution and cloud height become important. The analysis of these conditions requires different experimental approaches, of which visual method is the simplest. The visual method is subjective but more adequate for determining off-bottom solids suspension than for complete suspension. Due to the high cost of the equipment and the technical limitations, simulation techniques such as CFD can be employed for the same purpose [9–12]. To get insight into the influence of the hydrodynamics on homogeneity in such systems, detailed simulation and experimental data on the solid–liquid interaction is necessary.

Reactor geometry

Mixing tanks can have a flat or profile-based bottom, and the degree of the bottom curvature depends on the intended operation. Flat-bottomed stirred tanks are commonly used for liquid systems, while dished or elliptically bottomed tanks are used in solid–liquid or solid–liquid–gas systems to aid particle suspension. Many studies have been conducted in flat-bottomed tanks and with conventional impellers such as the Rushton turbine, pitched blade impeller and flat blade paddles [13–15]. Relatively few studies have been carried out with round or dished-bottomed tanks [16–18]. It is known that round bottomed tanks enhance particle suspension by eliminating dead zones at the wall junctions [18]. Dead zones or regions of segregation can be found at the wall junctions, especially for the high aspect ratio tanks with flat bottoms. The main advantages of the high aspect ratio tanks include high volumetric loading and economy of space, and the disadvantages are the increased regions of segregation and hydrostatic head. To reduce the dead zones in high aspect ratio tanks, the tank internals such as baffles and draft tubes are used [7]. Configurations of the high aspect ratio tanks deviate from the standard ones, in which the liquid height, H, is typically the same as the tank diameter, T, for a tank stirred by a single impeller. The standard impeller diameter, D, and its clearance from the bottom is $T/3$ [19]. Differences in the definition of the bottom impeller clearance with respect to the tank bottom profile and edge finishing accuracy may cause disparities in experimental results. Thus, many experimental data reported in the literature are not easily reproducible. However, a great deal of information can be generated if the experimental data is used to develop or validate the models.

EXPERIMENTAL METHODS AND EMPIRICAL MODELS

For many years, experimental methods of analyzing solid-liquid mixing focused on the bulk fluid flow [14,20,21] with a lot of attention being paid to the Reynolds number, *Re*. Many flows encountered in industrial processes are turbulent and the value of *Re* at which a system can be regarded as turbulent varies in the literature. A value of $Re > 10^4$ is generally considered to represent a turbulent flow [22]. However, Reynolds number does not account for the size or aspect ratio of the tank, which influences the distribution of the intensity of the turbulence in the tank. The fluid flow in tank regions closer to the wall and liquid surface may be laminar or turbulence, depending on the ratio of the impeller diameter to the diameter of the tank, impeller speed and the tank aspect ratio. The interaction between operating parameters and reactor geometry influences solid–liquid mixing features such as cloud height and off solids suspension. In the recent years, a lot of efforts have been devoted to the study of solids concentration distribution in stirred tanks [10,12,14,23,24]. Some of these studies have been conducted using non-intrusive techniques such as particle image velocimetry (PIV) and optical atenuation technique (OAT). Measurement and modeling of systems with high solids loading still pose a significant challenge.

Off-bottom solids suspension and cloud height

Solids suspension studies focus on three aspects: off-bottom solids suspension [20], solids cloud height [25] and solids concentration distribution [16]. The off-bottom solids suspension has been investigated in tanks stirred with single impellers [1,16,26] and with multiple impellers [23,24,27]. These systems provide different levels of homogeneity that may be required in a mixing tank, depending on the process. It is on this basis that the three aspects may be studied independently, or in relation to one another. In the case of crystallization and precipitation, for example, the rate of the reaction largely depends on the available surface area. For this reason, complete particle suspension is necessary.

Determination of the off-bottom solids suspension

One criterion that is typically used to investigate off-bottom solids suspension is the critical impeller speed, N_{js}, at which particles do not remain stationary at the bottom of the vessel for more than 1 to 2 s [20]. It has been reported [1] that N_{js} depends on both impeller clearance and the ratio of the impeller diameter to that of the vessel, D/T. Sharma and Shaikh [18] have shown that the response of the N_{js} to a change in the impeller clearance depends on the clearance range, and identified three different ranges. At a low clearance, there is an improved efficiency in energy transfer from the impeller to the solids, and the ratio of the local energy to the overall energy dissipation per unit volume is constant. The original form of the N_{js} correlation as developed by Zwietering [20] has limited application. The modification of this correlation by Sharma and Shaikh [18] enables its wider application to different tank configurations. More importantly, empirical constants in the correlations should represent meaningful aspects of the reactor configuration and the physics of the flow. The impeller induced fluid current is deflected by the tank bottom wall and subsequently drives the particles towards the liquid surface.

Cloud height

Bittorf and Kresta [25] developed a model that predicts the solids cloud height, which the authors defined as a well-defined interface that appears at the location where the downward velocity of the particles is exactly balanced by the upward velocity of the fluid at the wall. These authors [25] assumed that, once the particles have been lifted and prevented from settling, a force must move them away from the bottom and that this force depends on the wall jet. Therefore, their model was based on the relation between the solids cloud height and the maximum velocity in the wall jet, which is the flow created when fluid is blown tangentially along a wall. Ochieng and Lewis [11] developed a method of determining cloud height using OAT. The determination of the cloud height does not give any indication of the uniformity of the system and more information would still be required to determine the solids concentration distribution in the entire volume of the tank.

Solids axial concentration profile

Studies on the solids concentration distribution have been constrained by the cost of equipment required to obtain such data. Experimental methods have been developed to acquire data that is required to develop empirical or semi empirical models [14,16]. The quality of prediction obtained with these models depends on the accuracy of the experimental data. In such studies, the best computational fluid dynamics (CFD) simulation results are those that are validated using non-intrusive experimental techniques such as PIV and optical atenuation. Local solids concentration can be measured by a sampling method [2,16]. However, this is an intrusive method and the sampling probe may interfere with the liquid flow, causing measurement errors.

Measurement of solids concentration distribution

The less intrusive methods that have been used include, electrical resistance tomography (ERT) and positron emission tomography [28,29]. The ERT method is an imaging technique that can be used to map the electrical conductivity distribution that occurs in the system. Typically, the ERT method is employed in multiphase systems and the conductivity distribution is as a result of the phase distribution. The major limitation of the ERT method is that the interference with the bulk fluid flow increases as the number of measurement nodes increases. The size of the electrodes limits the number (typically 8-16) of planes along which measurements can be taken.

Fajner *et al*. [13] developed a very simple non-intrusive optical attenuation technique. This method and other methods based on the same principle have been employed to investigate solids concentration distribution [23,30,31]. In this optical method, light is transmitted across the tank by a light emitting diode and received on the opposite side of the tank by a silicon photo diode. The limitation of this method is that its accuracy decreases with an increase in solid hold-up and it can only be employed in a system where the tank is translucent. However, the experimental data obtain using such equipment may be used to develop models that can predict solid concentration in tanks that are non-translucent but can allow operation at elevated temperatures. In one of their most recent studies, Fajner *et al*. [32] employed the optical method to study solids concentration in a tank stirred using multiple impellers. However, these authors used a buoyant particle, for which the gravitation force does not have a direct influence on the particle distribution. Guha *et al*. [33] employed a computer automated radioactive particle tracking (CARPT) technique, which provides Lagrangian description of the solids flow field used to obtain the time-averaged velocity fields and the turbulent quantities.

Empirical models

The models that account for the concentration distribution are more informative than those that model the just off-bottom solids suspension or cloud height. Models based on the Peclet number (which is the ratio between convective flow and diffusion) and on dimensionless standard deviation, σ, of the actual solids concentration profile relative to vertical homogeneity have been used to predict the axial solids concentration profile [14,16,23]. Pinelli and Magelli [23] developed a one dimensional model, which is a reasonable approximation for flows in tall baffled tanks stirred by multiple impellers. However, this method lacks universality of application due to the three dimensional flow in stirred tanks. Montante *et al*. [24] pointed out that σ varies with tank configurations, operating conditions and fluid properties, and lacks physical significance. The limitations of the empirical models has been one of the motivations for the increasing interest in CFD.

CFD SIMULATION METHODS

The CFD simulation technique has developed very rapidly in the last fifteen years. The main aspects of the simulation strategies involve specifying boundary condition, grid size, discretization scheme, equation solvers, and turbulence and impeller models. Grid size and the governing equation are some of the major factors that influence the computational cost. Turbulence modeling influences both computational cost and the accuracy of the simulation results.

The application of CFD techniques in determining solid concentration distribution is rapidly increasing with the improvement in computer technology. In this context, one of the emerging multiphase simulation concepts applicable to systems with high solid hold up is the poly-disperse approach [12,18]. In this method, particle in a specific size range represent a phase. Ochieng and Lewis [12] further investigated the effect of particle size distribution of the solids concentration distribution.

Grid generation and boundary conditions

The primary objective of a simulation and modelling work is to accurately predict the performance of the real system and to show a trend in given process. Grid refinement can improve the accuracy of the simulation results, and it is desirable to obtain grid independent solutions. Grid independence studies should be carried at the preliminary stages before detailed definition of the solution strategy and the validation. For engineering design purposes, it is important to refine the grid to the extent that the simulation results are quantitatively and qualitatively comparable with experimental ones. For a grid independent solution, any further improvement in the accuracy obtained with a finer grid may not deserve the additional computational cost required. A summary of a sample of grid sizes that have been reported in the literature is given in Table 1. Detailed description of the grids distribution for a stirred tank model has been given by Montante *et al*. [34] and Ochieng *et al*. [35]. Finer grids are used in the regions of high turbulence and near the walls than in the rest of the tank.

Governing equations for solid-liquid mixing

In CFD simulation, the governing equations for a multiphase system can be described by the Langrangian [9,37,43] or Eulerian method [4,24,44]. The Eulerian method is sometimes referred to as a two-fluid model, with the fluids being treated as two interpenetrating media. The resulting turbulence momentum equations can be closed by the k–ε or other turbulence models. The Lagrangian method, on the other hand, treats one phase as continuous (described by the Eulerian equation) and the other as dispersed in a moving Lagrangian frame with Newton's second law of motion.

A summary of the literature review in Table 2 shows that there are little detailed CFD studies on solids concentration and particle size distributions. In particular, the data on solids concentration distribution for high density particles is very scarce [12,36,44]. Similarly, CFD studies on round bottomed tanks and the hydrofoil impeller are scarce due to the grid generation difficulties in many commercial software packages [18,44]. The problem was more severe with old CFD packages that that could generate only structured grids.

Lagrangian method

The large eddy simulation (LES) method and the Lagrangian approach for a 3D flow have been employed in dilute systems [3,43]. The Lagrangian approach reveals more detailed information on the trajectory of the particles in the tank than the Eulerian method. In the Lagrangian approach, only the velocity field is solved for, which is a valid approximation for low solid hold-up systems. However, as the solids loading increases, the resulting flow field depends on the interaction between the two phases. This interfacial interaction is not accounted for by this method, and the forces acting on the particles are based on correlations for single particles in unbounded flow. Moreover, the large number of particles to be tracked at high solids loading increases the computational cost considerably.

Eulerian method

Typically, the k–ε turbulence model is employed within the two fluid formulation context [50]. In this approach, the flow field is solved for both phases and the interaction between the phases is accounted for through the source terms. This approach has been employed in many studies reported in the literature [39,44,51,52]. Many researchers employ this method to simulate mono-size particles, and therefore, the influence of particle size on the solids suspension is not taken into account. Shah *et al*. [47,48] employed an Eulerian based poly-disperse multiphase simulation approach with six solid phases. However, very little quantitative information was given on the solids concentration distribution. Barrue *et al*. [9] employed the black box impeller modelling approach (IBC) to study solids suspension in a high solids volume fraction (20%) system. It has been reported that results obtained with the black box approach have limited application to other systems [53]. Ochieng and Lewis [12] employed poly-disperse approach to study solid concentration and particle size distributions for a high density (nickel) particles. These authors showed that the mono-disperse-particle assumption does not accurately represent the practical application, especially for high density particles. The high density particles tend to settle at the bottom of the tank. Further, it was shown that particle size distribution in the tank was dependent on the particle density and varied with both radial and axial dimensions of the tank.

Table 1. Grid size for the whole tank and system specifications

Reference	Grid size	Tank volume, L	*Re*	Impeller models
[36]	105,984	8.1	380	MFR[a], SG[b]
[12,13]	1,600,000	387	200-300	MFR, SG
[37]	162,590	13	2165	In-house
[38]	201,625	42	150-600	SG
[39]	208,000	21	360	IBC[c]
[40]	190,000	39	1020	SG
[41]	311,040	Not specified	50-150	MFR
[42]	216,000	2.5	1200-3000	MFR

[a]Multiple frame of reference; [b]sliding grid, [c]impeller boundary condition

Table 2. Experimental and simulation studies on solids distribution

Reference	Tank bottom	Impeller	Concept	Response variable	$\rho_p \times 10^3$ / kg m^{-3}	Method
[36]	Flat	RT	Conc. distrib.,	Vol. frac	2.58	CFD, LDV[a]
[11,12]	Round	Prop4	Conc. distrib., Cloud height	Vol. frac	9.8	CFD, LDV, OAT[b]
[3]	Flat	RT	Conc. distrib.	Vol. frac.	1.1	CFD
[22]	Flat	6 RTs	Conc. distrib	Vol. frac	2.4	OAT
[25]	Flat	PBI[c], A310	Cloud height	Jet Vel.	1.0–2.5	LDV, CFD
[1]	Round	PBI4	Off-Bot. Susp.	N_{js}[d], P[e]	1.3–1.6	Visual
[45]	Flat	–	Conc. distrib	Vol. frac	–	CFD
[4]	Flat	Lightnin A310, R100	Off-Bot. Susp.	N_{js}, P	2.6	CFD
[46]	Flat	PBI-U	Mixing	N_{js}, Nt_m[f]	0.84	CM[g], Visual
[8]	Flat	3 Propellers	Conc. distrib	Vol. frac	2.6	CFD, LDV
[47]	Flat	PBI6	Conc. distrib	Vol. frac	0.8–1.0	CFD
[48]	Flat	Prop4	Conc. distrib	Vol. frac	2.6	CFD
[39]	Flat	PBI4	Flow field	U_{slip}	8.9	CFD, PDV
[49]	Flat	RT	Off-Bot. Susp.	N_{js}, P	1–2.6	Visual
[40]	Flat	4PBI	Conc. distrib	Vol. frac	2.5	CFD, OAT
[2]	Flat	Marine	Piping	Mass fraction	2.65	Sampling
[1]	Flat	RT, PBI, FBT, HE3	Off-Bot. Susp.	N_{js}, P	2.5	Visual
[28]	Flat	PBI	Conc. distrib	N_{js}	2.4	ERT
[25]	Flat	6 RTs	Conc. distrib	Vol. frac	0.8–2.4	OAT
[16]	Dish	PBI	Conc. distrib	Vol. frac	2.6	Sampling
[13]	Flat	4 RTs	Conc. distrib.	Vol. frac	2.4	OAT

[a]Laser doppler velocimetry; [b]optical attenuation technique; [c]pitched blade impeller; [d]impeller speed at just off-bottom suspension; [e]power; [f]dimensionless mixing time; [g]conductivity meter

The typical CFD simulation method for investigating solids suspension is that the simulation is initiated with particles uniformly distributed in the domain. Such a simulation approach is likely to account only for the "avoidance of settling" mechanism and neglect the "bottom lifting" one. Both of these two mechanisms have been shown by Mersmann *et al*. [54] to be important for solids suspension. The simulation results obtained this way may not be easy to correlate to the classical methods for investigating solids suspension, such as the N_{js} approach. Kee and Tan [4] proposed a CFD simulation method to determine N_{js} in a flat-bottomed tank. In their method, the simulation was initiated with the particles at the bottom of the tank. However, the flow was only 2-D and the simulation results were not validated experimentally. The flow in a stirred tank is typically turbulent and three-dimensional and, therefore, a 2-D approach is a non-representative description of the complex flow in the stirred tank. Ochieng and Lewis [12] further explored this method in 3D geometries using high solids loading, and the simulation was initiated with particles initially settled at the bottom of the tank. The success of this method may depend on factors like drag curves and turbulence models. To verify this, Ochieng and Onyango [44] further explored the influence of drag curves on the simulation of solid concentration. The different drag curves used with the standard k–ε turbulence model produced similar results, with minor spatial variations.

Turbulence modelling

The turbulence models based on the Reynolds averaged Navier-Stokes (RANS) equations fall into two categories, namely, eddy-viscosity model and Reynolds–Stress models (RSM). The two-equation eddy-viscosity models include the renormalization group (RNG) k–ε, standard k–ε [55], and k–ω [56] models. For multiphase modelling additional terms are added to account for the interface momentum transfer.

The eddy-viscosity models are based on the assumption that there is an analogy between the viscous stress and Reynolds stress, and that the turbulent flow is isotropic [57]. The major weakness of the models based on the assumption of the isotropy of turbulence is that the predictions are less accurate in regions of anisotropic turbulence. Aubin *et al*. [58] reported that there was no significant difference between the predictions of the velocity field obtained with the k–ε and RNG k–ε turbulence models. A comparison between the RSM and eddy-viscosity models showed that RSM do not give better predictions of the turbulent and mean velocity field than the eddy-viscosity ones. Some studies [43,59] have shown that better prediction of mean velocity and turbulent fields can be obtained with the large eddy simulation (LES) approach. It has been suggested that further improvement may be obtained if the non-drag forces are accounted for [60].

Drag and non-drag forces

Drag is the dominant force in a system where one phase is continuous and the other one is dispersed. Non--drag forces, which include the turbulent dispersion, virtual mass, lift force the wall lubrication, may be accounted for depending on the fluid flow properties as well as particle and fluid physical properties [50,61].

Drag coefficients and models

There are different drag models available in CFD commercial packages, and these include the Schiller--Naumann, Ihme [62]; Ishii-Zuber [63]; Gidaspow [64], Brucato *et al*. [34] models. Ljungqvist and Rasmuson [39] compared the performance of the Ishii-Zuber, Ihme and Schiller-Naumann models against experimental results and reported that the predictions obtained with the three models were very similar. The authors made a further comparison between built-in models and the Brucato model and again reported that there was no difference in the results. The main difference between the Brucato model and the other models is that the Brucato model accounts for free stream turbulence. It can be noted that, except for the Gidaspow and Brucato models, the other models were developed for single particle immersed in a unidirectional flow. The fact that Ljungqvist and Rasmuson [39] did not observe any difference in the prediction with those models can be attributed to the fact that the λ/d_p ratio for their experiments was high enough so that C_D was not increased relative to C_{Do}. It therefore may not be an indication that the models give the same performance. The drag coefficient, C_D, which is the core parameter here, can be expressed by different correlations, depending on the system [62] as shown in Table 3.

The Gidaspow model [64] effectively becomes Wen-Yu and Ergun models for low ($\phi_s < 0.2$) and high ($\phi_s > 0.2$) solid hold-ups, respectively. The discontinuity at the crossover solids hold-up is taken care of by interpolating between Wen-Yu and Ergun over the range $0.7 < \varphi_L < 0.8$ [62]. The fluid drag coefficient for a quiescent liquid, C_{Do}, can be taken as C_D in Eq. (1) and λ is the Kolmogoroff length scale ($\lambda = (\nu^3/\varepsilon)^{1/4}$). Kolmogoroff hypothesised that there exists a range of eddy sizes between the largest and the smallest scale, for which the cascade process is independent of the statistics of the energy containing eddies [65]. The Kolmogoroff length scale, λ, which is a reference size of energy effective eddies is also a function of the kinetic energy dissipation rate, ε. Assuming uniformity of the kinetic energy dissipation rate, Brucato *et al*. [34] used the value of power dissipation per unit mass of fluid to compute the mean kinetic energy dissipation rate. However, this assumption did not account for the spatial variation of the turbulence intensity in a stirred tank. Montante *et al*. [40] employed the Brucato model with λ calculated by the same method described by Brucato and co-workers and further computed λ from the local turbulent kinetic energy dissipation rate determined from the CFD domain. These authors reported that there was no difference in the predictions by the two approaches. In principle, the CFD method is more representative of the spatial distribution of the turbulence intensity in the tank. However, this is only true if ε can be calculated accurately, which is not the case for RANS-based models [65,66]. The energy dissipation rate, ε, can be taken as the local turbulent kinetic energy dissipation rate, obtained from the CFD simulation.

The Brucato model has been employed in a dilute solid–liquid [39,40] systems: with solids volume loadings of 5% [40] and 0.001–0.02% [39]. In both systems, the model was reported to give a reasonable prediction of the solids concentration distribution. The free stream

Table 3. Drag models

Model	Expression	
Schiller-Naumannn	$\max(\frac{24}{Re}(1+0.15Re_p^{0.687}), 0.44)$, $Re_p = \frac{d_p U_r}{\nu}$	(1)
Brucato	$C_D = C_{Do}\left[1+8.76\times10^{-4}\left(\frac{d_p}{\lambda}\right)^3\right]$	(2)
Wen-Yu	$C_D = \phi_L^{-1.65}\max\left(\frac{24}{Re'_p}\left(1+0.15Re_p^{0.687}\right), 0.44\right)$, $Re'_p = \phi_L Re_p$	(3)
Ergun	$C_D = 150\frac{\phi_s^2\mu_L}{\left(1-\phi_s\right)d_P^2} + \frac{7\phi_s\rho_L\lvert U_r\rvert}{4d_P}$	(4)
Gidaspow	Eq. (3) for $\phi_s < 0.2$, otherwise Eq. (4)	

turbulence is accounted for by the Brucato model through the Kolmogoroff length scale. At high Reynolds number, there exists a separation of the length scales of the energy-containing eddies and inertial sub-range.

The main distinguishing feature of the Gidaspow model is that it is more suitable for the simulation of higher solids loading systems than the other drag models available in most CFD packages due to the fact that solids volume fraction is accounted for. Also, the model accounts for non-drag forces. A comprehensive evaluation of Gidaspow and Brucato has been carried out in both dilute and dense systems (1–20%w/w) [12,44]. The particles used by these authors were of high density (9800 kg/m^3) and they reported that the results obtained by both models were quite similar. However, it was pointed out that there were regions in the tank where, using both models, the experimental results were not well predicted. This short coming was attributed to the limitations of the turbulence models.

Non-drag forces

For most of the studies involving dilute systems, the influence of non-drag and solid pressure on solids suspension has generally been ignored. However, Ljungqvist and Rasmuson [39] and Sha *et al*. [47] investigated the influence of lift, virtual mass, and turbulent dispersion on slip velocity and observed that there was very little effect of these forces on the slip velocity. Ljungqvist and Rasmuson [39] studied solids suspension using very small nickel particles (75 μm diameter) in a dilute system for which the influence of the particles on the bulk fluid may not be significant.

Non-drag forces include the turbulent dispersion (F_{TD}), virtual mass (F_{VM}), lift (F_L) and wall lubrication (F_{WL}) forces. The turbulent dispersion force represents the effect of turbulent fluctuations on the effective momentum transfer. The virtual mass force is an inertial force, which is caused by the relative acceleration of the phases due to the movement of the particle [62]. The lift force denotes the traverse force caused by rotational strain, and the wall lubrication force tends to push the dispersed phase away from the wall. There are various versions of the non-drag forces and the turbulent dispersion force, and detailed descriptions of these forces are given by Lopez de Bertodano [50] and Lahey and Drew [61]. The way the turbulent dispersion force is accounted for depends on the averaging approach. For the time averaging approach, the turbulent dispersion force appears in the continuity equation as a function of the Schmidt number [40] and for Favre averaging, it appears as a force in the momentum equation [50,61,67]. Correlations to calculate these forces have been given in the literature [50,60,68]. Accounting for these forces has been reported to improve the accuracy of the simulation results [31].

Closure for solid-liquid turbulent flow

The forces representing the interaction between the phases need to be modelled in order to obtain closure for the resulting transport equations. The interfacial forces include the drag, non-drag and turbulent dispersion forces, of which the drag force is the most dominant. The coupling between the two phases is achieved by interphase coupling algorithms such as partial elimination algorithm (PEA) and simultaneous solution of non-linear coupled equations (SINCE). Interface coupling is incorporated into the mass balance pressure shared correlation step by the interface slip algorithm-coupled (IPSA-C) method. A detailed description of these algorithms is given by Karema and Lo [69]. Turbulence induced in the liquid phase by the particle can be accounted for through the turbulent viscosity by the model proposed by Sato and Sekoguchi [70].

The CFD simulation process starting from the grid generation all the way to closure of the transport equations sets the stage for data generation. The quality of the data depends on how well the models represent the real system. The data generated should aid process development and scale up. Already there is a large body of CFD knowledge on the physics of the fluid flow and more efforts are still required to couple the physical with the kinetics data. This will require increased application of large eddy simulations (LES) and direct numerical simulation (DNS) methods. The Euler-Euler and Lagrangian methods should be used complementarily rather than exclusively as each provide a unique set of information. Experimental methods are available to determine solids residence time distribution, however, CFD models to simulate this parameter are yet to be developed [71]. The application of CFD simulation to biological processes is rapidly increasing and will give a better insight into the important aspects such as the effect of shear stress on microbial growth.

CONCLUSION

This review has been carried on the application of the computational fluid dynamics techniques to simulate mixing in solid–liquid systems. The CFD models, which are based on the fundamental principles of transport phenomena, are more quantitative and predictive than the empirical ones which are largely system specific. The quantitative data is important for the design and analysis of hydrodynamics and mixing in stirred tanks. Many chemical reactions are carried out using stirred tanks, and the efficiency of such systems depends on the quality of the mixing, which has been a subject of research for many years. For solid–liquid mixing, the research efforts were traditionally geared towards determining mixing features such as off-bottom solid suspension using experimental methods.

In a few studies that focused on the determination of solids concentration distribution, methods that were used have not been accurate enough to account for some small scale mixing features such dead zones. Such features can now be accurately captured using CFD simulation techniques. The most reliable CFD simulation results are those that are generated from grid-independent data that are validated using high precision experimental techniques such as particle image velocimetry (PIV) and optical attenuation. Where there are disagreements between simulation and experimental data, especially in systems with high solids loading, there is an indication that the limitations of the turbulent models could be responsible for this. For this reason, more efforts need to be devoted to the use of large eddy simulation and direct numerical simulation methods in small scale systems, to reduce computational cost. This will create a strong foundation for the application of CFD simulation methods to concentrated solid–liquid mixtures, and for scale-up and process intensification.

The review shows that the increasing improvement in computer technology has made it possible to simulate biological systems that involve fermentation and biodegradation processes. This will provide more insight into the effects of hydrodynamics on reaction kinetics and product yield. In addition, there is a general trend towards the development of CFD simulation methods that predict particle trajectory, solids concentration distribution, particle size distributions which were traditionally determined using experimental methods only. Turbulence model still remains a major constraint in obtaining accurate CFD simulation data in many studies.

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IZVOD

CFD SUMULACIJA SUSPENZIJE ČVRSTIH ČESTICA U REAKTORU SA MEŠALICOM

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Predmet višegodišnjih istraživanja su mnogobrojne hemijsko reakcije koje se izvode korišćenjem reaktora sa mešalicom, pri čemu efikasnost ovih sistema zavisi od karakteristika mešanja. Za mešanje čvrsto–tečno, korišćenjem eksperimentalnih tehnika napori istraživača su obično usmereni ka određivanju osobina mešanja, kao što su čvrste suspenzije iznad dna. U nekoliko istraživanja koja su se bavila određivanjem raspodele koncentracije čvrste suspenzije, neke korišćene metode nisu dovoljno tačne za objašnjenje nekih „zloćudnih" pojava kao što je postojanje mrtvih područja (dead zone). U ovom preglednom radu prikazana je primena Proračunske dinamike fluida (engl. *computational fluid dynamic*, CFD) za simulaciju osobina mešanja, kao što su čvrste suspenzije iznad dna, koncentracija čvrste materije, raspodela veličine čestica i visina „oblaka". Podaci o dejstvu veličine čestica i raspodele veličine čestica na raspodelu koncentracije čvrste materije su još uvek oskudni. Napredak CFD modelovanja je usmeren ka sprezanju fizičkih i kinetičkih podataka radi razumevanja mešanja i reakcije na mezo- i mikro-skali. Raspodela vremena zadržavanja čvrste materije je važna za projektovanje. Ipak, postojeći CFD modeli ne predviđaju ovaj parametar. Poslednjih godina, postignuti su izvesni pomaci u primeni CFD simulacije na sisteme koji uključuju fermentaciju i anaerobne procese. U ovim sistemima, složeno uzajamno dejstvo između biohemijskih procesa i hidrodinamike još je nedovoljno jasno. Ova je jedna od oblasti koja zahteva dalja istraživanja.

Ključne reči: CFD • Mešanje • Višefazni tokovi • Simulacija • Čvrsta suspenzija
Key words: CFD • Mixing • Multiphase flows • Simulation • Solid suspension