*Symposium on Computational Modeling of Metals, Minerals and Materials, TMS Annual Meeting, February 17-21, 2002, Seattle, WA.*

# CFD MODELING OF SOLIDS SUSPENSIONS IN STIRRED TANKS

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## Abstract

An understanding of the parameters that govern the just-suspended impeller speed, $N_{js}$, and the distribution of solids, is critical to the efficient operation of hydrometallurgical and other processes involving solid-liquid suspensions. In this paper, the distribution of solids in stirred tanks under a range of solids loadings (0.5 to 50 vol%) was predicted using CFD and validated against experimental data obtained from the literature. The multiphase flow is modeled using the Eulerian Granular Multiphase model. This paper will also review the established design parameter $N_{js}$ in the context of scale-up and compare it to the quality of solids dispersion as a means of assessing correct scale-up in suspension tank design. The results of this study will describe a straightforward procedure to obtaining comprehensive information about reactor behavior with complex CFD models.

The performance of hydrofoil impellers and a 45° pitched-blade turbine at suspending solids under different agitation speeds was studied. Both single and dual impeller operation have been evaluated. The settled solids fraction for speeds below $N_{js}$, and the cloud height for impeller speeds above $N_{js}$ were predicted. The CFD predictions are in good agreement with experimental literature data on velocity distribution and cloud height.

## Introduction

Mechanical agitation is widely used in process industry operations involving solid-liquid flows. The typical process requirement is for the solid phase to be suspended for the purpose of dissolution, reaction, or to provide feed uniformity. If these vessels are not functioning properly, by inadequately maintaining suspension, the quality of the products being generated can suffer. Associated with the operation of these units is a need to maintain the suspension at the lowest possible cost. The challenge is in understanding the fluid dynamics in the vessel and relating this knowledge to design. Computational Fluid Dynamics (CFD) modeling can provide insight to both the multiphase transport and the design parameters. Recent advances in CFD allow for the modeling of multiphase systems, such as the liquid-solid mixtures discussed here. There are a variety of approaches to modeling the solids transport and include Lagrangian or homogenous techniques with the liquid phase influencing the particle motion but not the particles influencing the liquid (one-way coupling). Of particular interest is the Eulerian multiphase model, which uses separate sets of Navier-Stokes equations for the liquid and solids (or granular) phases. In this approach, the interactions between the phases are coupled. Recent work (1) predicted particle distributions of low particle concentrations in single and multiple impeller stirred vessels using Eulerian-Eulerian models. Their simulations were in reasonably good agreement with experimental axial measurements of solid concentration. However, some uncertainty in the results predicated the authors to use correction factors to fit the numerical predictions to experimental data. Their conclusions were that improved single-phase simulations and incorporation of so-called four-way interactions (fluid-particle, particle-fluid, particle-particle, and particle-turbulence interaction) would improve the applicability and reliability of the modeling work. The Eulerian Granular Multiphase (EGM) model (2) provides a fully predictive solution of the solids transport in the process vessel. The EGM model accounts for four-way coupling between and within the phases that applies to systems with dense granular flows. The strongly coupled momentum equations of the granular and liquid phases require a transient solution. The application of Eulerian Granular multiphase (EGM) model to modeling solids suspension in stirred tanks has not been reported in the literature.

In this paper we will elucidate the criteria of minimum suspension speed and it's prediction using the EGM model, validate the CFD predictions of solids distribution with experimental data, and evaluate scale-up criteria for stirred tanks suspending solids. The focus of this paper is to present a methodology that can allow engineers and experts alike to predict performance of agitation systems used for solids suspension. The paper will address the suspension of freely settling solids occurring in typical processes that involve dissolution, reactions, and feed uniformity. Slowly settling materials such as pulp suspensions and biosludges that exhibit complex rheology due to interaction in the suspension phase were not considered.

## Characterizing the Suspension Solids in Stirred Tanks

<u>Just-suspended speed</u>

Historically, the characterization of the suspension of solids in stirred tanks is through the parameter of the just-suspended speed $N_{js}$. The concept of $N_{js}$ was introduced more than forty years ago and is the primary design parameter used today by engineers involved in the sizing, scaling and overall design of stirred tanks for the purpose to suspending, dissolving and reacting solids. The famous correlation by Zwietering (3) correlates the $N_{js}$ to the particle and fluid properties, the mass ratio percentage of the solids, and the impeller diameter. The parameter $S$ in the Zwietering correlation incorporates the influence of the tank bottom shape, impeller clearance and blade characteristics. This lumped parameter can be evaluated from tables developed by many workers and scattered over the literature. $N_{js}$ has generally been estimated experimentally in laboratory scale vessels in a subjective manner and the reliability of the correlation on scale up to industrial mixers has been questionable. Alternative methods of computing $N_{js}$ have been proposed (4,5) and require the determination of a parameter(s) relating to the number, type and clearance of the agitator. Some correlations were developed with a narrow range of impeller blade styles, sizes and position in laboratory scale tanks and as such the large variability in predicting $N_{js}$ for industrial scale vessels may or may not be acceptable. For CFD analysis, the criterion that solid particles remain motionless on the bottom of the vessel for less than 1-2 seconds is meaningless from a mathematical standpoint. Using CFD to predict $N_{js}$ is an optimization problem that would be computationally expensive and not practical as the D, C and N would be varied for a specified impeller and tank diameter. An alternative criterion for characterizing solids suspension is needed.

Cloud Height

In suspending solids, the level of agitation is the primary parameter for design. Increasing the agitation level takes the suspension from a state of motion to complete suspension to uniform distribution. The $N_{js}$ determines the transition to complete suspension but criteria for determining complete suspension are not available. The cloud height is related to the agitation level in the vessel. Vigorous agitation well above the $N_{js}$ will distribute the cloud of solids. The uniformity of the distribution can be considered the quality of suspension. Consider the three systems from Bakker *et al.* (6) in Figure 1 that are all operating above $N_{js}$. Each system shows a different level of solids distribution. It is interesting to note that the cloud height is not uniform across the tank diameter as the simulations show the funneling of the solids being drawn towards the impellers. The 3D CFD results qualitatively predict the extent of the solids distribution in the tanks.

If one were to integrate the concentration of the solids over the vessel, one would come up with the average concentration and relative standard deviation of concentration. The relative standard deviation $\sigma$ would represent the quality of the suspension. Recently (7), the quality of suspension was correlated to the Froude number and impeller clearance as a means of characterizing the extent of solid suspension (see Figure 2). For uniform suspension: $\sigma < 0.2$, for just-suspended condition: $0.2 < \sigma < 0.8$, and for incomplete suspension: $\sigma > 0.8$. From a numerical standpoint, the quality of suspension is a more quantitative evaluation of the distribution of solids.

## Modeling Liquid-Solid Multiphase Flow

There are a number of multiphase models that can be used to model the solids suspension in an agitated vessel. The Lagrangian Eulerian model solves the equation of motion for the discrete particle trajectories. The coupling between the phases through drag terms can be modeled but accumulation of particles cannot be modeled. The drift flux and ASM models are homogeneous mixture models for modeling multiphase flows. The ASM model introduces slip between the phases through an algebraic relationship. These models are ideally suited to modeling particles with relaxation times less than 0.001-0.01 seconds and in low concentrations. The Eulerian models are the most rigorous of the multiphase models and model the multiple phases as interpenetrating continua. A separate set of momentum equations is solved for each phase. The interaction between the phases is modeled through the momentum exchange terms and includes the drag exerted by the continuous phase on the dispersed phase. In the EGM model, the granular momentum equation includes in a solids stress tensor that is modeled based on the kinetic theory for granular flow described by Gidaspow (8). An additional transport equation for granular temperature (or solids fluctuating energy), which is proportional to the mean square of the random motion of particles, is modeled.

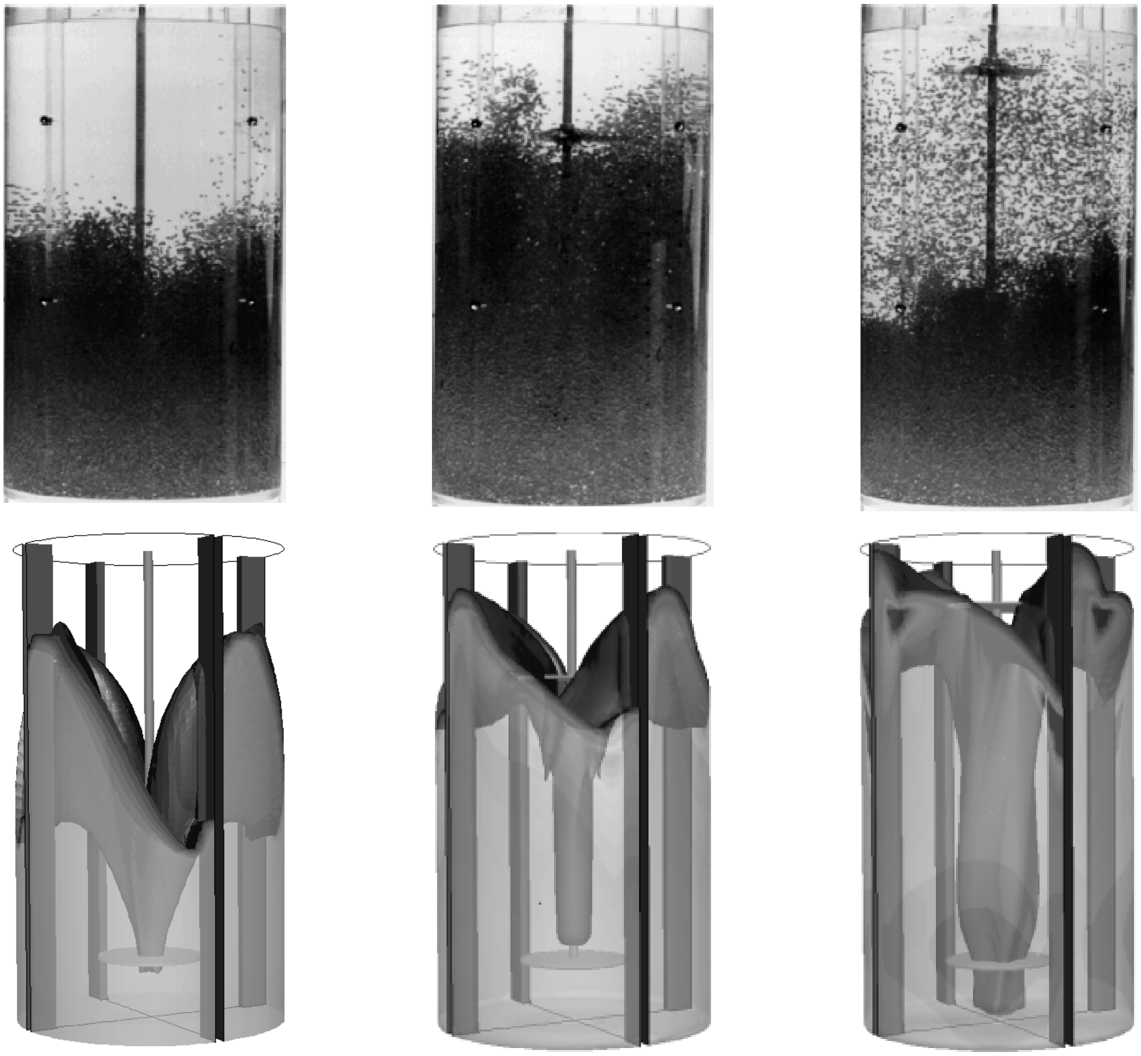


Figure 1: Three systems operating above $N_{js}$ but exhibiting different cloud heights and varying degrees of solids suspension.

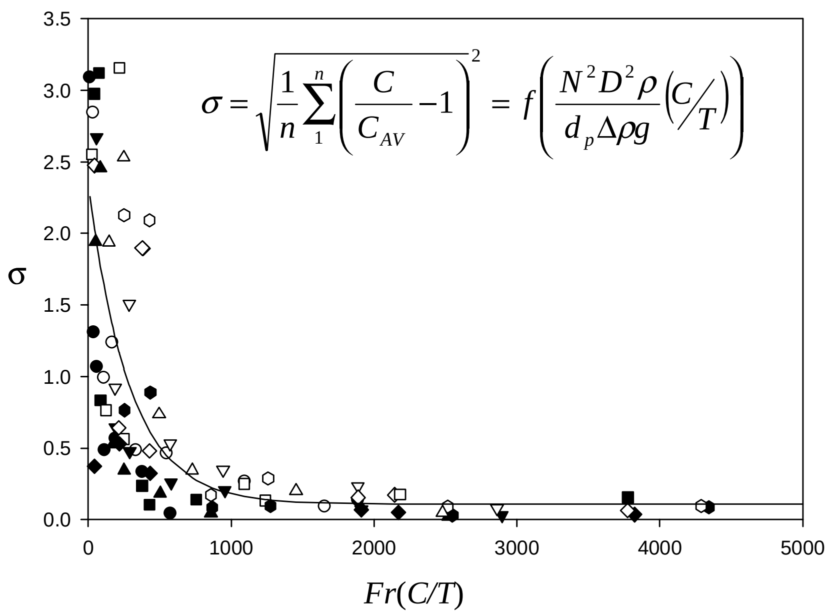



Figure 2: The relative standard deviation or so-called "quality of suspension" of solids concentration as a function of Froude number and impeller clearance.

Numerical Methods and Boundary Conditions

The stirred tank models (computational grids of quad or hex elements) were set-up automatically using MixSim from Fluent Inc. (9). The commercial CFD code FLUENT 4.52 was used with the EGM model in the solution of the solid-liquid multiphase flows. The granular viscosity model of Syamlal & O'Brien (10) was used in this work. The fluid-solid exchange coefficient correlation of Di Felice *et al.* (11), developed for the drag on particle suspensions, was used. Turbulence in the liquid phase was modeled using the standard k-ε model and secondary phase turbulence generation was neglected. The EGM model calculations are performed as time-dependent.

No-slip boundary conditions ($u$=$v$=$w$=0) for both phases are applied on the tank walls and shaft with the latter having a prescribed rotational velocity. The free surface of the suspension is described by zero gradients of velocity and all other variables. Since the shear stress is zero, the free surface can be interpreted as a slip wall. The impellers were modeled implicitly using internal boundary conditions based on laser Doppler velocimetry (LDV) data supplied by the impeller manufacturers. LDV impeller data can also be obtained from a number of sources (12). The impellers can also be modeled explicitly in three-dimensions using the multiple reference frames or sliding mesh models but add to the computational expense of the calculations.

Due to the simplicity of the mixing tank geometry and the explicit treatment of the impellers, the stirred tanks were set up as 2D axisymmetric models with a transport equation for swirl. To account for the presence of the baffles, the tangential velocity is reduced to zero in the baffle region. By modeling the mixing tank in two dimensions, the simulation runtime is considerably accelerated. The computational grids consisted of approximately 3,000 cells in the 2D models. Larger three-dimensional models were also set up for comparison. After obtaining the continuous (liquid) phase steady-state flow field, the time-dependent solids suspension calculations were performed. Typically, the multiphase flow field reached "steady-state" after 120 seconds. Typical calculations took about two hours of CPU time (Sun Ultra 60 300MHz or Intel Pentium 450MHz) to produce 60 seconds of real process time. Experimental data from the literature was chosen to validate the two-phase flow field for (1) *the velocity distribution*, (2) *the distribution of solids in the stirred tank, and*, (3) *the influence of the solids on the mixing time.*

## Two-Phase Velocity Distribution

Experimental LDV measurements from Guirard *et al.* (13) were used for comparison with the CFD simulations. The stirred tank geometry and liquid and solid property data are listed in Table I. Figure 3(a) shows the flow field produced in the stirred tank where the vectors represent the liquid velocity magnitude. The flow is highest near the impeller and is relatively low near the free surface. The distribution of solids in the tank is shown by the contours of solids volume fraction in Figure 3(b). Note that the impeller speed of 306 rpm is much greater than $N_{js}$ of 106 rpm computed from the Zwietering correlation. The relative standard deviation of solids volume fraction is 0.57 and reflects the lack of complete suspension in the tank observed in Figure 3(b). The black contour level represents the clear liquid layer above the solids cloud.

Table I: Tank, impeller and material properties from Guirard *et al.* (13)

| Geometry | Properties | |
|---|---|---|
| 3 blade Hydrofoil Impeller<br>D/T = 0.47; C/T = 1/3<br>N = 5.1 rps<br>T = H = 0.3 m | Liquid | $\rho$ = 1000 kg/m$^3$<br>$\mu$ = 1cp |
| | Solids | $\rho$ = 2230 kg/m$^3$<br>$d_{50}$ = 253 $\mu$m |

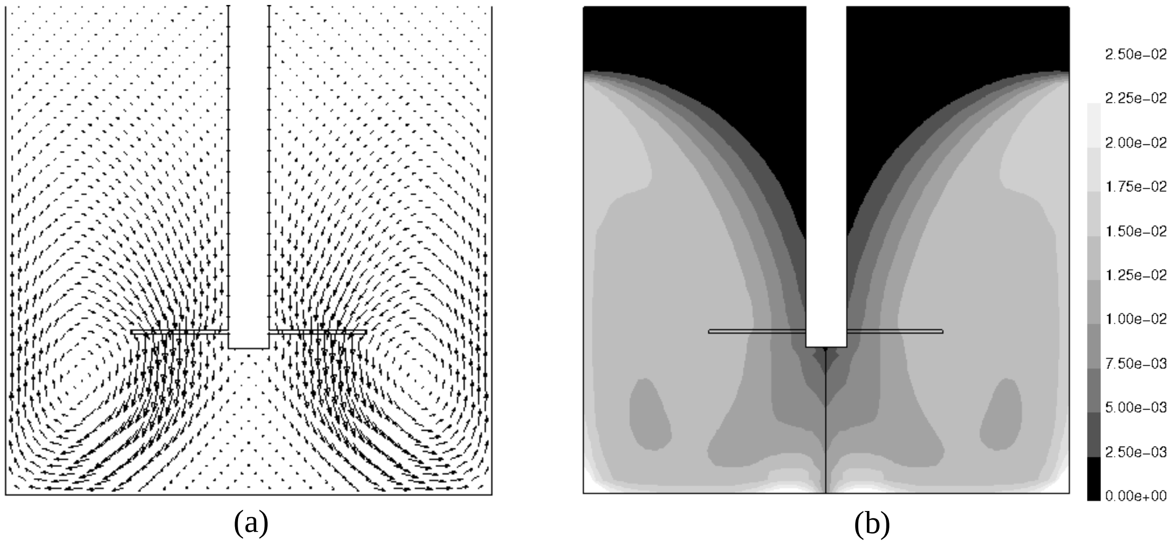



Figure 3: Flow field for dilute (0.5vol%) suspension (a) Liquid phase flow field with range of velocity magnitude from 0 - 0.85 m/s (b) Volume fraction contours of the 253 μm solids represented where σ was calculated as 0.57.

Figure 4 shows good agreement between the predicted and measured axial velocity. The axial velocity measurements were made at *r/D* of 0.464 and 0.961, mid-way between the baffles. The solids and continuous phase velocities differ as expected and this difference is captured in the numerical results. Due to slip between the phases, the solids velocity lags the continuous phase velocity particularly near the impeller. Near the top of the tank, the continuous phase velocity slows and the settling of the particles due to gravity produces a higher axial velocity in the solids phase. In Figure 4(b), the agreement with the experiments is poorer since the measurements where made between baffles near the tank wall. The 2D simulation circumferentially averages the flow field between the baffles resulting in a smoother velocity profile.

## Axial Solids Concentration Profiles

Measurements of the axial distribution of solids concentration by Godfrey & Zhu (14) were considered for validation in this paper. A summary of the stirred tank geometry and liquid and solid property data are listed in Table II. Figure 5 shows the flow field and volume fraction distr-

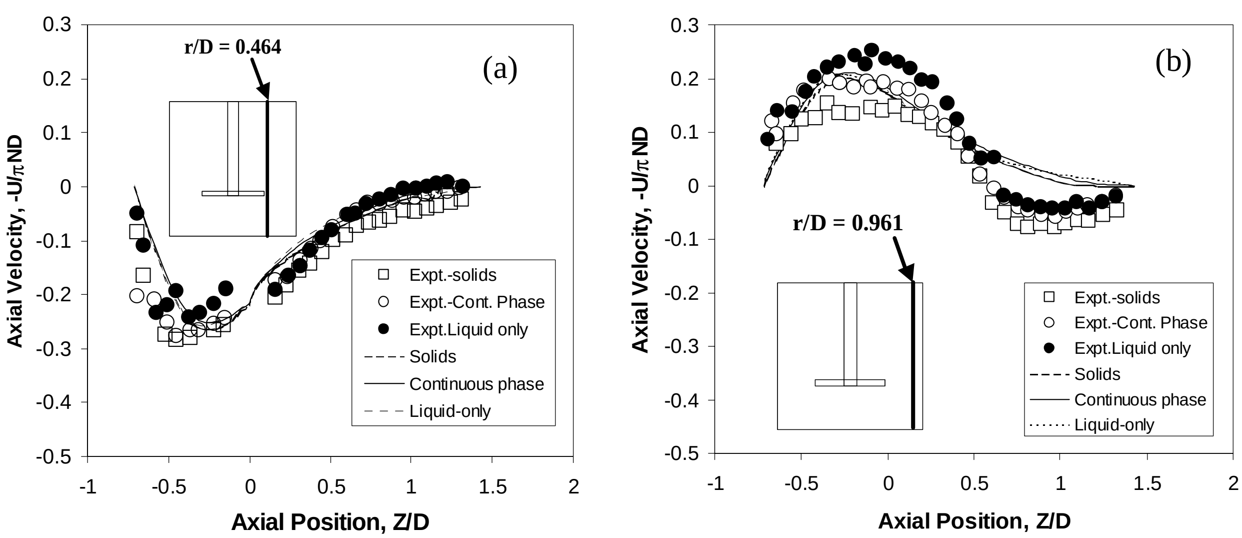



Figure 4: Single- and two-phase axial velocity profiles at *r/D* of 0.464 and 0.961 in mid-baffle plane as a function of height. Experimental data from Guirard *et al.* (13)

Table II: Tank, impeller and material properties from Godfrey and Zhu (14)

| Geometry | Properties | |
|---|---|---|
| 4PBT45°<br>D = T/3; C = T/5<br>N = 1000, 1600 rpm<br>T = H = 0.154 m | Liquid | $\rho = 1096$ kg/m$^3$<br>$\mu = 1.76$ cp |
| | Solids | $\rho = 2480$ kg/m$^3$<br>$d_{50}$ = 231, 390μm |

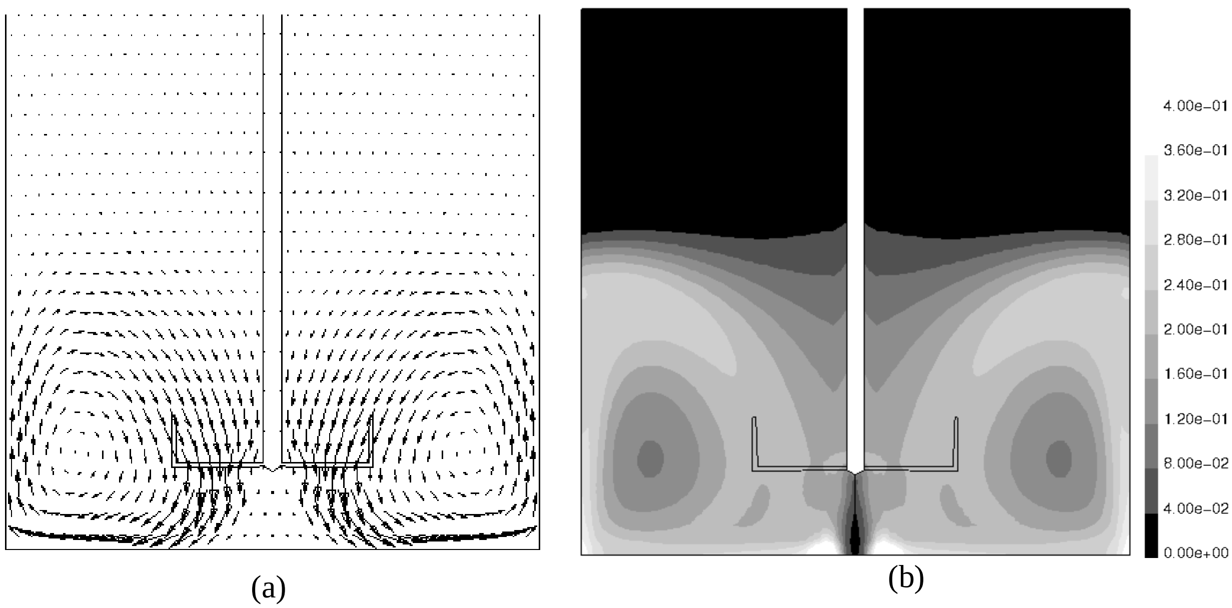



Figure 5: Flow Field Distribution at N = 1000 rpm and 390 μm particles (a) Liquid flow field vectors: 0 - 0.95 m/s (b) Solids Volume Fraction with $\sigma = 0.87$ showing the cloud height just past mid-way up the tank.

ibution of 390 μm particles in the tank with an agitation speed of 1000 rpm. The $N_{js}$ from Corpstein (4) was determined to be 780 rpm and from Zwietering was 1170 rpm. The quality of suspension was 0.87, which indicates that the agitation speed of 1000 rpm is not sufficient to satisfy the just-suspended criterion. The influence of agitation speed and particle diameter on the axial distribution of solids concentration will be discussed next.

<u>Effect of Agitation Speed</u> Figure 6(a) shows the axial profiles of normalized solids concentration X (local solids concentration/average solids concentration, the average solids concentration was 12vol%) for 390 μm particles at 1000 and 1600 rpm agitation speeds. The solids concentration measurements were made mid-way between the impeller and the baffle. Both the 2D and 3D CFD predictions of the solids concentration profiles are in good agreement with the experimental measurements and the cloud height is predicted correctly. At the lower agitation speed, the solids are not completely suspended and a cloud height forms as shown by the transition in the axial concentration profile. The height of the particle cloud coincides with the change in direction of the single-eight flow pattern (see Figure 5(a)). The high velocity in the loop transports the bulk of the solids with lower solids concentration in the center of the loop (see Figure 5(b)). This is the reason the axial solids concentration profile goes through the transition below the cloud height as shown in Figure 6. The CFD predictions are less dispersive than the experiments and tend to exaggerate the variation in the axial profile of solids concentration through the single-eight flow loop established by the axial pumping PBT. Although Godfrey and Zhu did not quantify the experimental error in their data, which would contribute to part of the deviation, the

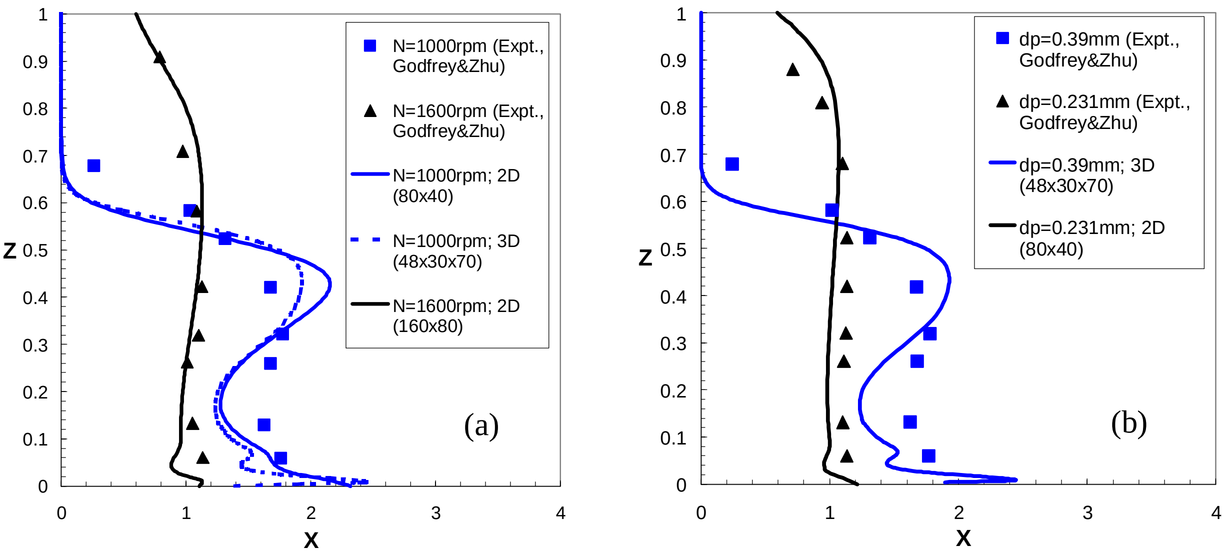



Figure 6: Axial distribution of solids concentration (a) Influence of agitation speed (Particle diameter of 390 μm) (b) Influence of particle diameter (Agitation speed of 1000 rpm). Experimental data from Godfrey and Zhu (14).

solution of separate turbulence equations for the solids phase could perhaps improve the prediction by increasing the turbulent dispersion of the solids phase.

As the agitator speed is increased to 1600 rpm, the suspension becomes more homogeneous or completely suspended and no appreciable transition in the axial concentration profile is observed. For the low clearance, axial pumping agitators that create high gradients of velocity in the flow field impinging on the vessel bottom, care must be taken to refine the grid resolution near the bottom and side walls to improve the accuracy of the simulations.

<u>Effect of Particle Diameter</u> Figure 6(b) shows the axial profiles of normalized solids concentration X (local solids concentration/average solids concentration, the average solids concentration was 12vol%) for 231 and 390 μm particles at an agitation speed of 1000 rpm. There is good agreement between the predictions and the experimental measurements. As the particle diameter decreases, the drag and slip velocity decrease allowing the solids phase to be transported more easily by the continuous phase increasing the dispersion of solids in the tank. Therefore, by reducing the particle diameter, at constant impeller speed, the suspension becomes more complete.

## Influence of Solids on the Mixing Time in the Liquid Phase

The influence of dense solids concentration on the blending of the continuous liquid phase was investigated by Bujalski *et al.* (15). It was observed that when the solid particles are fully suspended but have a clearly defined cloud height, the mixing time may be two or more orders of magnitude longer than in the single-phase case. The tank, impeller and material properties selected for comparison with CFD predictions are listed in Table III. The mixing time of the liquid phase was determined experimentally using the decolorization technique. The mixing time is the time required for the uniformity $U$ of tracer concentration ($U = 1 - [C_\infty - C(t)]/C_\infty$), measured at multiple locations in the tank, to reach within 1% of the equilibrium concentration. The details of the method for simulating mixing time using CFD are described by Oshinowo *et al.* (16).

Table III: Tank, impeller and material properties from Bujalski et al. (15)

| Geometry | Properties | |
|---|---|---|
| Lightnin A310<br>D/T = 0.52<br>C/T = 1/4<br>N = 300 rpm<br>T = H = 0.29 m | Liquid | $\rho$ = 1000 kg/m$^3$<br>$\mu$ = 1 cp |
| | Solids | $\rho$ = 2500 kg/m$^3$<br>$d_{50}$ = 115μm<br>$C_{av}$ = 25, 50% |

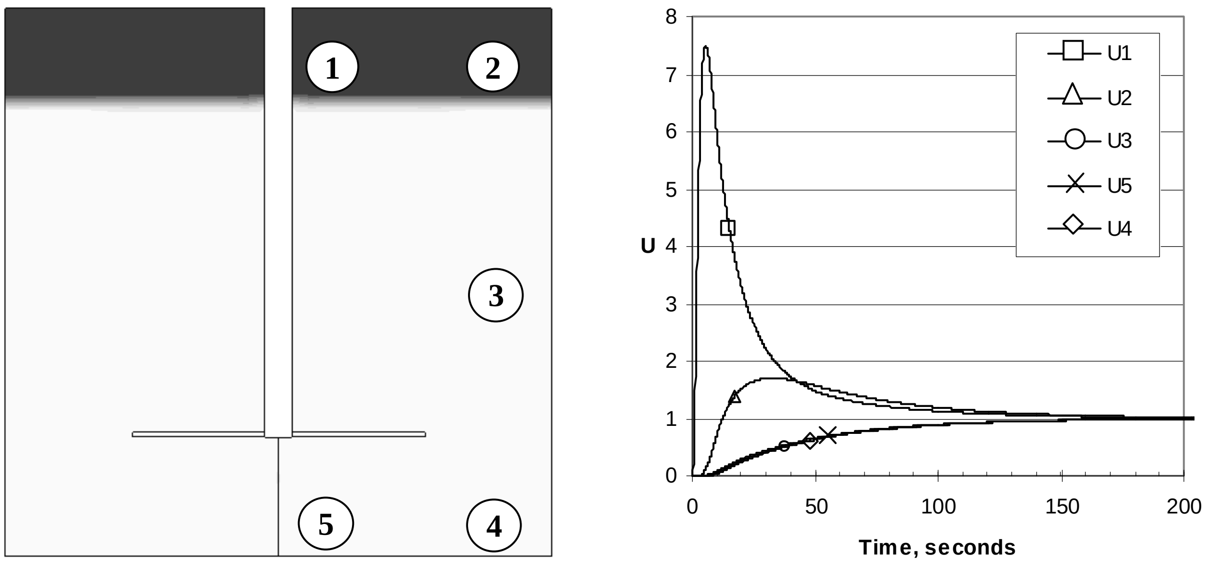
Table IV: Comparison between CFD and experimental measurements of mixing time $Nt_m$ in the liquid phase of the dense solid-liquid suspension.

| | **Relative Mixing Time $(Nt_m)/(Nt_m)_{water}$** | |
|---|---|---|
| **Solids Concentration** | **Experiments** | **CFD** |
| 25 vol% | 4.2 | 5.8 |
| 50 vol% | 21 | 17 |

Table IV compares the CFD predictions of mixing time with the experimental results from Bujalski *et al*. (15) The tracer was introduced just below the free surface near the drive shaft. The mixing time in water $(Nt_m)_{water}$ was determined from CFD to be 13 seconds. The agreement is good and is well within the experimental error of the decolorization method used to determine the mixing time. The mixing time in the solids suspension is much higher than in water alone and increases with solids concentration. In particular, at the operating agitation speed of 300 rpm, the solids are almost fully suspended forming a clear layer in the upper part of the tank (see Figure 7(a)) The predicted flow pattern is in agreement with the experimentally observed $N_{js}$ of 329 rpm with the Zwietering correlation overpredicting $N_{js}$ at 410 rpm. The weak flow in the clear layer coupled with slow transport of the tracer across the interface inhibits the blending process as shown by the concentration measurements at the sample locations in Figure 7(b). The uniformity in the clear layer, indicated by U1 and U2 in Figure 7(b), is higher than unity early in the blending process due to the initially higher local tracer concentration in the clear layer, although all sample locations reach equilibrium concentration at approximately the same time.

## Scale-up Criteria for Solids Suspension

Despite much research, the problem of how to scale-up solids suspension systems has not been completely solved. Zwietering suggested a scale-up exponent of -0.85, which results in a decreasing power input per unit volume when the system is scaled up. Corpstein et al. (4) refined this further by linking the scale-up exponent to the particle settling velocity, which addressed the problem of the seemingly inconsistent values for the scale-up exponent found in the literature. Later, unpublished work by the same researchers suggested that the scale-up exponent is also affected by scale itself, although to a much lesser degree than it is affected by particle settling velocity. Furthermore, it was observed in experiments that the scale-up exponents for just-suspended speed and to obtain the same relative cloud height were actually different. This would point to the conclusion that the scale-up methods used to predict $N_{js}$ are not necessarily suited for predicting the solids distribution uniformity in the vessel, which is the main parameter predicted by CFD. This is illustrated by the following example: The system described in Table II was scaled by a factor of 6.5. The $N_{js}$ for original and new size was 1170 and 236 rpm, respectively, based on Zwietering's correlation. The quality of suspension was determined by CFD to be 0.86 and 0.72, for the original and new size, respectively. This shows that the scale-up based on $N_{js}$ alone is insufficient to determine the quality of the suspension. It is clear that additional research




(a) (b)

Figure 7: Blending in a high solids concentration (50vol%) suspension. (a) Volume fraction of solids showing clear layer of water at top of tank and near uniform solids suspension below. (b) Tracer uniformity at the five sample locations shown in (a).

is needed to address the issue of the different scaling methods that are apparently needed for $N_{js}$ and suspension uniformity.

## Conclusions

A practical application of CFD to model the low to high concentration solids suspensions in stirred tanks and predict the distribution of solids, the velocity distribution of the solids and liquid, the cloud height of the suspension, and the blending of the liquid phase, has been described in this paper. The agreement with experimental data from the literature was very good. The just-suspended speed correlation was shown to be inconsistent in determining the $N_{js}$ for the tank systems evaluated. It is possible that the low clearances combined with modern high efficiency impellers require addition modification to the original $N_{js}$ correlation. However, the standard deviation of solids volume fraction was shown to be useful measure of the quality of suspension. Further work to develop a general relationship for the quality of suspension is in progress. Based on the methodology described in this paper, process design and analysis can be rapidly performed to scale geometry, evaluate tank modifications, such as, baffling and draft tubes, and the agitator performance in hydrometallurgical or similar applications can be evaluated rapidly.

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