

## CFD PREDICTIONS OF SOLIDS DISTRIBUTION IN STIRRED VESSEL

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### ABSTRACT

This paper presents a CFD model for predicting solid particle distribution in a stirred tank. The tank is operated at the “just suspended” condition, which is difficult to model due to the high variation of solid concentration within the vessel. The concentration of solid particles is high near the base of the vessel and low at the top near the free surface. The ability to predict the “just suspended” condition is very important in industrial applications as it determines the lowest power input necessary to suspend the solid particles.

In this work the Eulerian Multiphase Model implemented in STAR-CCM+ is used to simulate suspension of glass particles in a stirred vessel. The turbulent flow is modelled using the standard k-ε model. The drag force acting on the particles is modelled using the Gidaspow formula. Two modelling techniques: Multiple Reference Frame (MRF) and Rigid Body Motion (RBM) also known as the sliding grid method are used for the impeller rotation. RBM correctly resolves the impeller-baffle interactions and gives a better prediction of the flow field but is more computationally expensive in comparison to the MRF method.

CFD predictions of the local solid concentrations and velocities are compared against the experimental data of Guida et al. (2009) for a single PBT impeller. Two solids concentrations of 5.2% wt and 10.6% wt and two impeller pumping modes are considered. The comparisons are made in terms of accuracy and computational time.

### NOMENCLATURE

$A$	constant in solid pressure force equation
$A_{ij}^D$	linearized drag coefficient
$c$	concentration of solid particles
$C_D$	drag coefficient
$d$	particle diameter
$D$	impeller diameter
$g$	gravitational acceleration
$F$	force
$m_{ij}$	mass transfer rate to phase $i$ from phase $j$
$M_i$	interphase momentum transfer
$N$	impeller speed
$N_{js}$	impeller speed for “just suspended” conditions
$p$	pressure
$S$	constant
$S_i^\alpha$	source term in mass balance
$\mathbf{v}$	velocity
$\mathbf{v}_r$	relative velocity between phases
$X$	solid loading

$\alpha$	volume fraction
$\rho$	density
$\mu$	dynamic viscosity
$\nu$	kinematic viscosity
$\nu_c^t$	turbulent viscosity
$\sigma_\alpha$	turbulent Prandtl number
$\tau_i$	stress tensor

### INTRODUCTION

The suspension of solid particles in a stirred vessel is a key requirement in a number of industrial processes including the production of pharmaceuticals, fine chemicals, paper and food products. The distribution of solid particles determines both the final product quality and the process efficiency by affecting mass transfer and reaction rates.

The solid suspension is usually characterized by two parameters, the impeller speed that corresponds to the just suspended condition and the cloud height. The “just suspended” condition corresponds to the lowest impeller speed at which solid particles do not stay at the vessel base longer than 1 second. The just suspended condition also corresponds to the lowest power input necessary to suspend solid particles. The cloud height defines the position of the interface between the suspended solids and the clear liquid at the top of the vessel.

Traditionally the just suspended condition is estimated based on empirical correlations e.g. Zwietering (1958) correlation:

$$N_{js} = S V^{0.1} \left[ \frac{g(\rho_d - \rho_c)}{\rho_c} \right]^{0.45} X^{0.13} d^{0.2} D^{-0.85} \quad (1)$$

In order to use the above correlation the proportionality constant  $S$ , which is geometry dependent, has to be known and that limits the applicability of this correlation to typical impeller systems.

In this work we use Computational Fluid Dynamics (CFD) to predict the solid distribution in a stirred tank. This approach allows arbitrary impeller geometry to be modelled and gives deep insight into the solid suspension process.

### MATHEMATICAL MODEL DESCRIPTION

In this work the Eulerian multiphase flow model implemented in STAR-CCM+ was used to model the distribution of solid particles in the stirred tank. The Eulerian multiphase model treats the liquid and solid phases as interpenetrating continua. Each phase is

characterized by its own physical properties and velocity. The pressure is shared by the phases and the amount of a given phase in the computational cell is given by the phase volume fraction.

STAR-CCM+ solves mass conservation equation for phase  $i$ :

$$\frac{\partial}{\partial t}(\alpha_i \rho_i) + \nabla \cdot (\alpha_i \rho_i \mathbf{v}_i) = 0 \quad (2)$$

and momentum equation takes the form:

$$\frac{\partial}{\partial t}(\alpha_i \rho_i \mathbf{v}_i) + \nabla \cdot (\alpha_i \rho_i \mathbf{v}_i \mathbf{v}_i) = -\alpha_i \nabla p + \alpha_i \rho_i \mathbf{g} + \nabla \cdot [\alpha_i (\boldsymbol{\tau}_i + \boldsymbol{\tau}_i^t)] + \mathbf{M}_i + (\mathbf{F}_{\text{int}})_i \quad (3)$$

Where the turbulent stresses  $\boldsymbol{\tau}_i^t$  are given by the k- $\epsilon$  model taking into account the extra source terms arise from the presence of the interfacial forces in the momentum equations.

The momentum equation accounts for two interfacial forces: drag force and turbulent dispersion force and the solid pressure force in the solid phase equation.

#### Solid pressure force

The presence of solid particles results in additional solid pressure force that needs to be added to the momentum balance. The solid pressure force takes into account particle-particle interactions when the solid volume fraction is close to the maximum packing limit. In this work an exponential formula was used:

$$(\mathbf{F}_{\text{int}}) = -[e^{A(\alpha_d, \max - \alpha_d)}] \nabla(\alpha_d) \quad (4)$$

(STAR-CCM+ User Guide 2012).

#### Drag force

The Gidaspow formula is used for the drag force. It connects the Ergun equation for high solid particle concentration with a modified Stokes law for regions of low or moderate concentrations. The linearized drag coefficient  $A_{ij}^D$  is given by:

$$A_{ij} = \begin{cases} \frac{150\alpha_d^2 \mu_c + 1.75\alpha_d \rho_c |v_r|}{\alpha_d d^2} & \alpha_d \geq 0.2 \\ \frac{3}{4} C_D \frac{\alpha_d \rho_c}{d} |v_r| \alpha_c^{-1.65} & \alpha_d < 0.2 \end{cases} \quad (5)$$

where  $C_D=0.44$  and the drag force is given by:

$$\mathbf{F}_{ij}^D = A_{ij}^D (\mathbf{v}_j - \mathbf{v}_i) \quad (6)$$

#### Turbulent dispersion force

The turbulent dispersion force accounts for the interaction between the dispersed particles and the surrounding turbulent eddies. Following formula is used:

$$\mathbf{F}_{ij}^{DT} = A_{ij}^D \frac{v_c^t}{\sigma_\alpha} \left( \frac{\nabla \alpha_j}{\alpha_j} - \frac{\nabla \alpha_i}{\alpha_i} \right) \quad (7)$$

where  $\sigma_\alpha$  is the turbulent Prandtl number equal to 1. The turbulent dispersion force is important in predicting the cloud height as pointed out by Lo (2006).

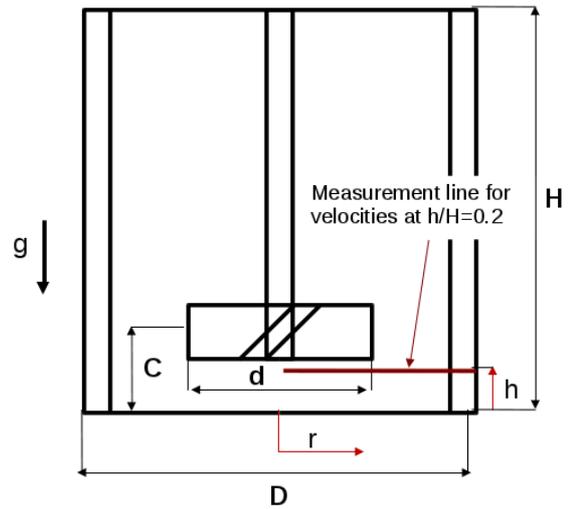
#### Impeller rotation models

The impeller rotation is modelled using two approaches, moving reference frame (MRF) and rigid body motion (RBM). In the MRF model, the grid is stationary and two different reference frames are used, stationary and rotational. This approach is approximate and provides good results when interactions between the rotor and stator are weak. The MRF model can be used in steady-state simulations as it does not require the grid movement. In contrast, the RBM model moves the rotor grid with respect to the stator grid hence the impeller-baffle interactions are modelled directly. It is more accurate in most of the simulated cases, but it requires a transient simulation and small time step that correctly resolves the grid movement.

#### EXPERIMENTAL WORK OF GUIDA ET AL.

The CFD model was validated against the experimental data of Guida et al. (2009) for a single PBT impeller. Two solids concentrations 2.5% vol, and 5.2% vol and two impeller pumping modes were considered.

The experimental system is schematically shown in figure 1.

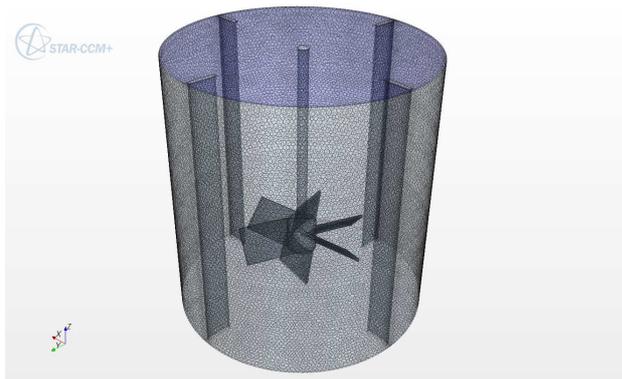


**Figure 1:** Schematic diagram of experimental system.

The tank diameter was 0.3m, the liquid level equalled to the tank diameter. A 6-blade 45-deg PBT impeller with diameter 0.15m was used. The tank has a flat base and fitted with 4 standard baffles. The liquid used was a salt solution in water with a density of 1150 kg/m<sup>3</sup>. The dispersed phase consisted of glass particles with an average diameter of 3.075 mm. The measurements were performed using positron emission particle tracking technique.

#### CFD MODEL

A CFD model of Guida's vessel was created in the STAR-CCM+ software. The whole geometry was modelled. The computational grid was build using polyhedral elements as shown in Figure 2.



**Figure 2:** Grid used in the simulations.

The grid dependency study was carried out for grids 300k cells up to 1.1M cells. The solution was grid independent. The grid with 488k cells was used in the simulations. The grid was constructed in such a way that the grid was finer near the impeller to resolve high gradients. All boundary conditions were set to walls except the top of the tank that was modelled as a symmetry plane. A slip wall could be used to represent the free surface at the top boundary. Turbulence damping would be represented by the slip wall and not the symmetry plane, however, the difference between the two approaches on the results presented here is small because the measurement plane is relatively far from the top boundary.

The same grid was used for MRF and RBM calculations with the interface between rotation and stationary zones placed half way between the impeller tip and the baffles.

The MRF model was run in steady state whereas the RBM model was run in transient.

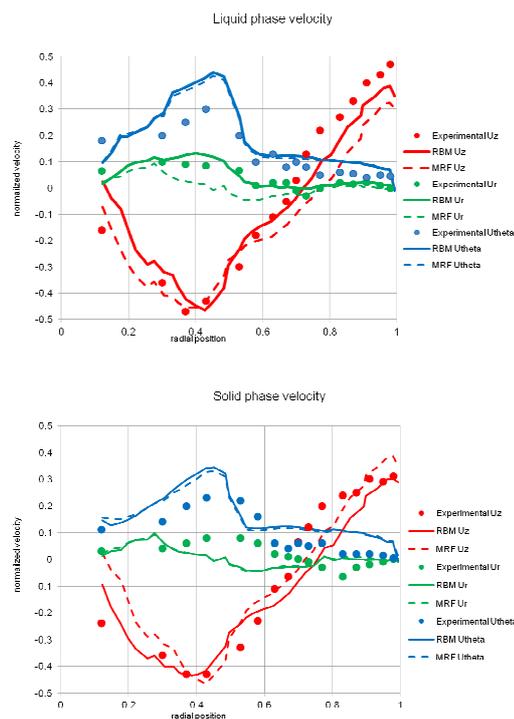
Second order discretization schemes were used. The convergence criteria were based on the normalized residuals to drop below  $10^{-4}$ .

The simulations were initialized with uniform distribution of solid particles.

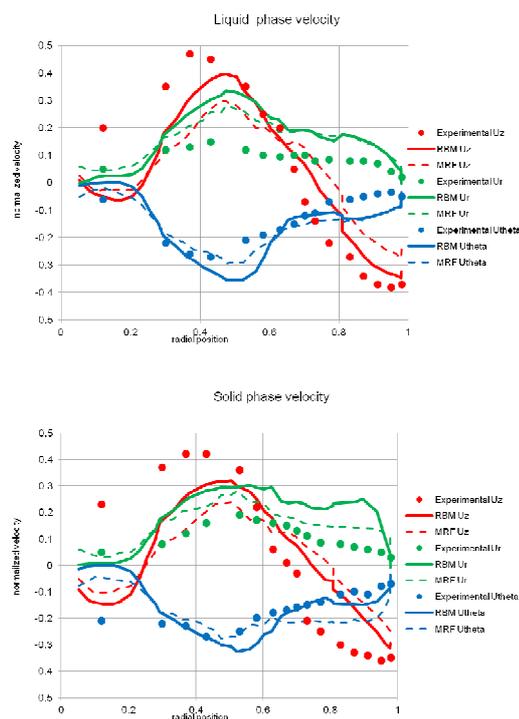
## CFD RESULTS

Two solid particle concentrations were modelled, 2.5% (vol) and 5.2% (vol). The predictions of solid phase and liquid phase velocities are given in figures 3-6. The velocities were measured at the plane located at the discharge of the impeller ( $h/H=0.2$  for down-pumping impeller and  $h/H=0.4$  for up-pumping impeller). The velocities for the RBM model were averaged over 5 impeller revolutions because after 5 impeller revolutions no further changes in average quantities were observed.

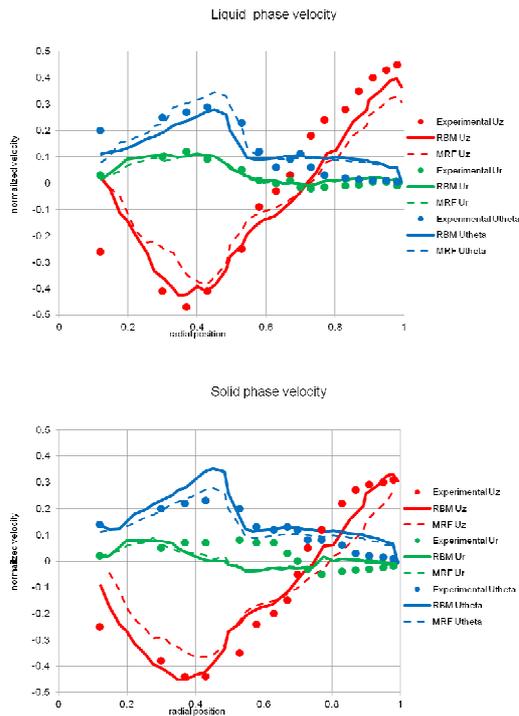
Figures 3-6 show the comparison of velocity predictions for two particle concentrations and two impeller pumping modes.



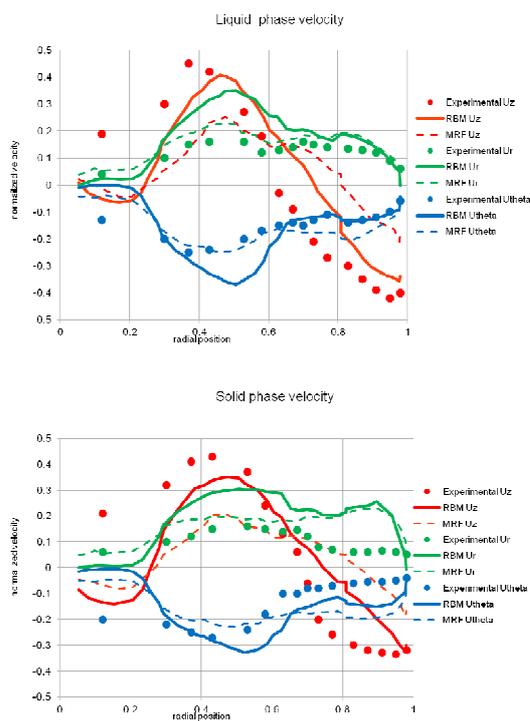
**Figure 3:** Liquid phase and solid phase velocities for 2.5% vol,  $N=360$  rpm, down-pumping



**Figure 4:** Liquid phase and solid phase velocities for 2.5% vol,  $N=375$  rpm, up-pumping



**Figure 5:** Liquid phase and solid phase velocities for 5.2% vol, N=405 rpm, down-pumping



**Figure 6:** Liquid phase and solid phase velocities for 5.2% vol, N=410 rpm, up-pumping

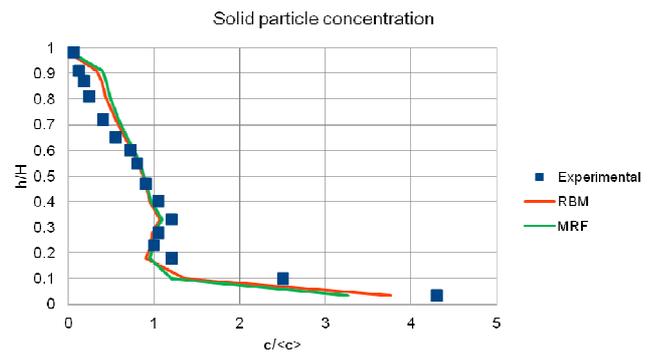
The results show that RBM and MRF model gives similar results.

On average the steady state MRF model took 18 times less time to solve than the transient RBM. For MRF model, the converged solution is reached after 4000 iterations whereas RBM requires to resolve 4 seconds of the flow field that gives about 80,000 iterations.

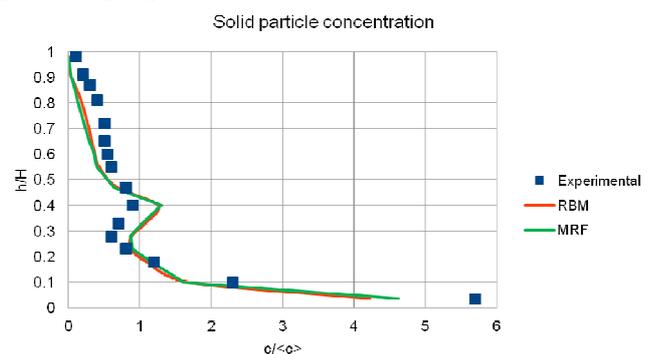
The differences in velocity profiles between experimental data and CFD predictions can be attributed to limitations of the standard k- $\epsilon$  model. For example Joshi et al. (2011a, 2011b) gives extensive comparison of different turbulence models and predictions for the single phase flow near the impeller by k- $\epsilon$  models show significant error. In this work only standard k- $\epsilon$  model was used as it is still commonly used in engineering applications.

CFD model gives better prediction of the flow pattern at the impeller discharge if the impeller operates in down-pumping mode. One possible reason could be the measuring plane is directly underneath the impeller. In down-pumping mode the measuring plane is close to the impeller, the source driving to the flow. Since the impeller is modelled explicitly, the flow generated by the impeller is fairly well represented by the CFD model. On the other hand, in up-pumping mode the measuring plane is close to the end of the returning flow back to the impeller. This returning flow is complicated by the mixing, turbulent and flow pattern in the rest of the tank. The weaknesses of the turbulence model are amplified in this case. The up-pumping cases are therefore more difficult to predict well at the chosen measuring plane.

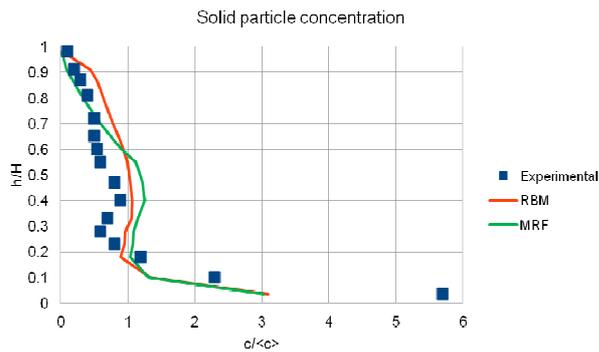
Figures 7-10 show the distribution of solid particles in the tank for two particle concentrations and two impeller pumping modes.



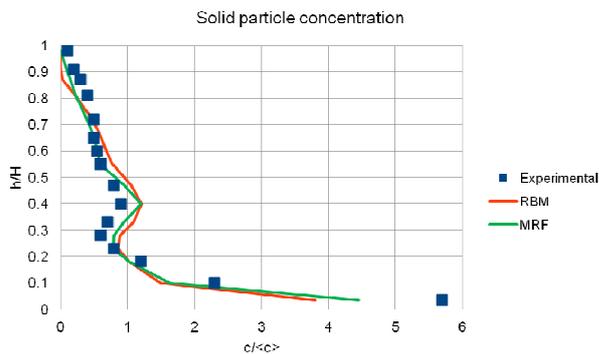
**Figure 7** Solid particle concentration for 2.5% vol, N=360 rpm, down-pumping



**Figure 8** Solid particle concentration for 2.5% vol, N=375 rpm, up-pumping

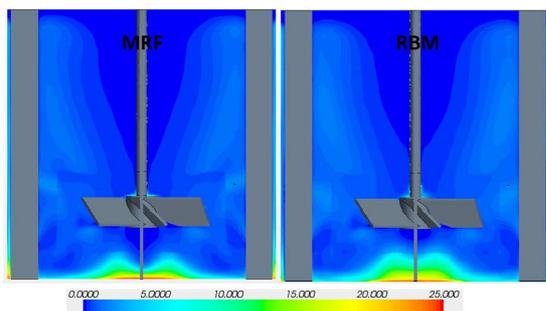


**Figure 9:** Solid particle concentration for 5.2% vol, N=405 rpm, down-pumping



**Figure 10:** Solid particle concentration for 5.2% vol, N=410 rpm, up-pumping

In all cases CFD model is close to experimental data. The CFD model correctly predicts the cloud height and distribution of solid particles. The RBM model and the MRF model give similar results. Figure 11 shows that there is a small difference in solid volume fraction below the impeller caused by different rotation model. The RBM model seems to be slightly less diffusive allowing a higher concentration of particle to accumulate below the impeller.



**Figure 11:** Contour profiles of solid particle concentration for 2.5% vol, N=360 rpm, down-pumping

## CONCLUSION

The results presented in this paper show that CFD model can correctly predicts the distribution of solid particles in a stirred vessel.

CFD predictions of velocity profiles show good agreement when the impeller is operated in the down-pumping mode but not so good in the up-pumping mode. The reason

could be in down-pumping mode the measuring plane is recording the fairly well defined flow discharged from the impeller, whereas in the up-pumping mode the measuring plane is recording the returning flow back to the impeller after been through the complex turbulent mixing flow in the tank.

In down-pumping mode, the RBM model does not significantly improve the velocity prediction indicating that turbulence modelling is a source of error as shown by Joshi et al. (2011a and 2011b).

The MRF model offers similar accuracy to the RBM model and requires on average 18 times less computational time.

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