CHISA 2002
Prague, 25-29 August 2002

CFD PREDICTIONS OF SOLID CONCENTRATION DISTRIBUTIONS IN A BAFFLED STIRRED VESSEL AGITATED WITH MULTIPLE PBT IMPELLERS

Giuseppina Montante[1], Donato Rondini[1], André Bakker[2], Franco Magelli[1]

[1]Dipartimento di Ingegneria Chimica, Mineraria e delle Tecnologie Ambientali
Università di Bologna - Viale Risorgimento 2 - 40136 Bologna (Italy)
Tel. +39 051 2090406, Fax +39 05106347788, E-mail: giusi.montante@guest.ing.unibo.it

[2]Fluent Inc., 10 Cavendish Court, Lebanon, NH 03766, USA

ABSTRACT

In the present work the predictive capabilities of CFD techniques as applied to solid-liquid stirred vessels are investigated. The distribution of solid particles was simulated in a high aspect-ratio baffled stirred tank agitated with three Pitched Blade Turbines (PBT). Suspensions of glass beads of diameter equal to 327 μm and 675 μm in water were studied. The mentioned geometric configuration for the vessel was chosen for the simulations as the solid distribution profiles offer a challenging benchmark for the solid-liquid simulation approaches.

The simulations of solid-liquid suspensions in the baffled vessel were performed by using fully predictive approaches. A Eulerian-Eulerian and a Eulerian-Granular multiphase models were adopted for modelling of the solid-liquid flow coupled with the “mixture”, “dispersed” and “for each-phase” k-ε models. The two-phase simulation techniques employed are described. The simulated particle axial concentration profiles are compared with the experimental data and critically discussed.

1. Introduction

The distribution of solid particles is one important feature of solid-liquid stirred tanks whose experimental behaviour has been mainly described with simple fluid-dynamic models over the years. Very dilute solid-liquid suspensions have been considered in most experimental investigations.
More recently, also CFD methods have been applied to the simulation of solid-liquid stirred tanks and different models have been developed for predicting the behaviour of the solid phase (Bakker et al., 1994; Decker and Sommerfeld, 1996; Barrue et al., 1999; Sha et al., 1999; Micale et al., 2000; Montante et al., 2001; Ljunqvist and Rasmuson, 2001; Brucato et al., 2002), either based on Lagrangian or Eulerian approaches. The need for further analysis and development of modelling techniques and comparison of the simulations with experimental data arises from several reasons. Black box methods for the treatment of baffled stirred tanks were often adopted, thus leading to not entirely predictive procedures. In addition, a number of modelling techniques have been proposed and implemented in

commercial codes, whose choice is not straightforward for the normal user. Moreover, the consistency of the simulation predictions with the actual flow field and solid particle distribution has been demonstrated only in few cases.
In the present work, both experimental and computational analyses were performed in a baffled tank agitated with a down-pumping Pitched Blade Turbine (PBT), with solid average concentration up to 4% by volume. A high aspect-ratio vessel was selected that gives rise to particularly pronounced vertical solids concentration gradients, thus providing a rather severe test for solid particle dispersion models.
The multiphase and turbulence models available in the CFD code Fluent 6.0, coupled with fully predictive impeller simulation strategies, have been tested in order to find out which of the different modelling techniques may lead to the most satisfactory representation of the flow field and solid distribution in solid-liquid stirred vessels.
As a difference with our previous work, the technique adopted for these experiments allowed to measure the local particle concentration, thus permitting additional tests on the radial profiles. Also, one-order-of-magnitude solids loading bigger than in the past (e.g. Montante et al., 2001) was investigated.

2. Experimental

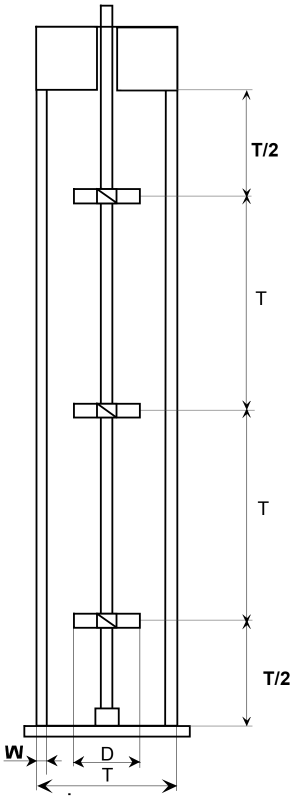

Figure 1 Vessel geometrical configuration.

The experimental data were collected in a cylindrical, flat-bottomed tank of diameter T= 0.48m and height H=3T. The vessel, depicted in Figure 1, had a lid and was equipped with four vertical T/10 baffles. Agitation was provided with three equally spaced 4-blade 45° PBT of diameter D=0.195 m. The lower impeller was at the distance T/2 from the base; impeller spacing was equal to T.
The liquid used was water at room temperature. As the solids, mono-sized spherical glass particles of diameter d_P=327 and 675 μm were used. The mean solids concentration was 10-15 and 100 grams per litre. The impeller speed was N=8.07 s^{-1}, i.e. higher than the "just suspended" condition.
The solids concentration distribution in the tank was determined by means of an optical probe that provided local measurements. The probe, depicted in Figure 2, was cylindrical (0.8 cm in diameter) and encased two optical fibres connected to a diode and a photodiode; a small mirror fixed perpendicularly to the probe axis at a distance of 2.4 cm from the fibre tips defined the optical path for the measurement. The probe was inserted horizontally in the vessel through lateral ports at 35 elevations; at each elevation four radial measurements were taken – except at the turbine level were only the two outer positions were accessible.

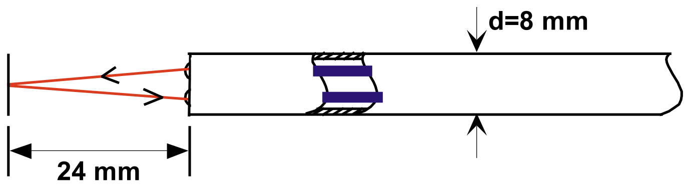

Figure 2 The probe for local measurements.

3. CFD simulations

The CFD simulations of the stirred tank described above were performed by adopting two different mathematical models, namely Eulerian-Eulerian and Eulerian-Granular, both based on an Eulerian treatment of the two phases. With these approaches, the continuity and momentum equations are solved for each phase, thus obtaining separate flow field solutions for the liquid and the solid phases simultaneously.
The continuity and momentum equations for a generic phase q, based on the Eulerian treatment, are:

$$\frac{\partial}{\partial t}\left(\alpha_q\right)+\nabla\cdot\left(\alpha_q\vec{v}_q\right)=0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\alpha_q\rho_q\vec{v}_q\right)+\nabla\cdot\left(\alpha_q\rho_q\vec{v}_q\vec{v}_q\right)=-\alpha_q\nabla p+\nabla\cdot\overline{\overline{\tau}}_q+\vec{R}_{pq}+ \\ +\alpha_q\rho_q\left(\vec{F}_g+\vec{F}_{lift,q}+\vec{F}_{vm,q}\right) \tag{2}$$

where α_q is the volumetric fraction of the phase q, F_g is the gravitational force and F_{lift} and F_{vm} are the lift and virtual mass force, respectively. These last two forces have been neglected in the calculations, as it was already found that they give a minor contribution to the solution with respect to the other terms (Ljunqvist and Rasmuson, 2001). The inter-phase momentum transfer term, R_{pq}, is modelled *via* the drag coefficient, C_D, as:

$$R_{sl}=\frac{3}{4}\frac{\alpha_s\rho_s}{d_p}C_D\left|\vec{v}_s-\vec{v}_l\right|\left(\vec{v}_s-\vec{v}_l\right) \tag{3}$$

This last parameter was calculated by using the standard correlation implemented as a default in Fluent 6.0 (Schiller and Nauman, 1933) that refers to a particle falling in a still fluid. Also, the effect was investigated of a correction to take into account the increase in the drag coefficient due to free stream turbulence (Magelli et al., 1990; Brucato et al., 1998).
The Granular model differs from the Eulerian one for the momentum equation of the solid phase, that is modified with respect to Eqn (2) as:

$$\frac{\partial}{\partial t}\left(\alpha_s\rho_s\vec{v}_s\right)+\nabla\cdot\left(\alpha_s\rho_s\vec{v}_s\vec{v}_s\right)=-\alpha_s\nabla p-\nabla p_s+\nabla\cdot\overline{\overline{\tau}}_s+F_g+ \\ +K_{ls}\left(\vec{v}_l-\vec{v}_s\right)+\alpha_s\rho_s\left(\vec{F}_s+\vec{F}_{lift,s}+\vec{F}_{vm,s}\right) \tag{4}$$

As can be observed, this equation is identical to the previous one (2), except for one additional term that introduces a "solid pressure" contribution. This term has been modelled according to the kinetic theory of granular flows (Ding and Gidaspow, 1990) as implemented in Fluent 6.0.

In the present case of turbulent two-phase flow, the momentum transfer due to the turbulent fluctuations of the volumetric fraction is taken into account by adding to both Eqn (3) and (4) the additional term:

$$R_{sl}^{t} = \frac{3}{4}\frac{\alpha_s \rho_s}{d_p} C_D \left| \vec{v}_s - \vec{v}_l \right| v_{dr} \tag{5}$$

where the drift velocity, v_{dr}, is defined as:

$$v_{dr} = \frac{D_s}{\sigma_{sl}\alpha_s}\nabla\alpha_s - \frac{D_l}{\sigma_{ls}\alpha_l}\nabla\alpha_l \tag{6}$$

In Eqn (6), D is the turbulent diffusivity and σ is the turbulent Schimdt number.

In order to close the problem, a suitable turbulence model has to be coupled with the Reynolds Averaged Navier-Stokes equations. Three different extensions of the standard k-ε model to multiphase systems have been developed.
In the simplest case, referred to as "Mixture Model", only a couple of k and ε equations are solved, where the physical properties of the mixture are adopted; therefore, the two phases are assumed to share the same k and ε values.
A more advanced modification of the single phase k-ε model, named "Dispersed Turbulence Model", is based on the solution of the k and ε equations for the liquid phase, while the turbulence quantities for the solid phase are calculated on the basis of a simplified treatment (Tchen, as quoted in Hinze, 1975).
The most rigorous turbulence model includes a set of k and ε equations for each of the phases (thus called "For Each Phase Model") and allows taking the turbulent transport of the flow variables into account.
The relevant equations of the mentioned turbulence models are not reported here for the sake of brevity, as they can be found elsewhere (Fluent Inc., 2001).

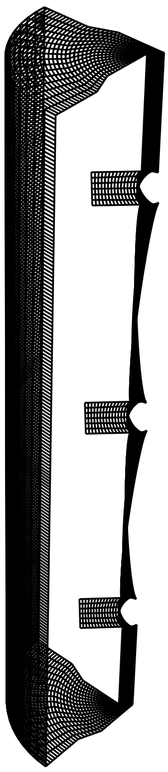

Figure 3 Computational grid.

The models described above were coupled with the Multiple Reference Frame (MRF) simulation strategy. The MRF allows simulating baffled stirred tanks, without requiring any experimental input, by subdividing the whole vessel in two cylindrical computational domains, that is an external domain containing the baffles and an inner one containing the impeller. As a difference with other fully predictive approaches, in the MRF the stationary RANS equations are solved, thus neglecting the periodicity of the flow field. Nevertheless, this approach has been chosen on the basis of previous findings (Brucato et al., 2002) showing that the spatial solid distribution is not significantly improved when transient approaches are employed (that are much more computationally expensive).

The computational grid adopted for all the simulations is shown in Figure 3 and consisted of 116640 cells: 178x37x16 along the axial, radial and tangential coordinates, respectively. In the present case of 4 impeller blades and 4 baffles, it was possible to limit the azimuthal extension of the domain to $\pi/2$; periodic boundary conditions in the azimuthal direction were imposed. The simulations were started from still fluid conditions and particles uniformly distributed in the computational volume. Finally, the computational domain was partitioned in three sub-domains and the parallel version of Fluent 6.0 was run on a three-processor computer.

4. Results and discussion

4.1 Experimental results

In Figure 4 (a), (b) a few of the experimental radial concentration profiles are depicted for the particles of mean diameter d_p=675 (a) and 327 µm (b). The solid average concentration was of 100g/L in both cases. As can be observed from the profile at the lower elevation, the minimum concentration is closer to the vessel wall in the case of the bigger particles, probably because of the higher inertia of those particles; the radial distribution is flatter and flatter going towards the vessel top for both particle size.

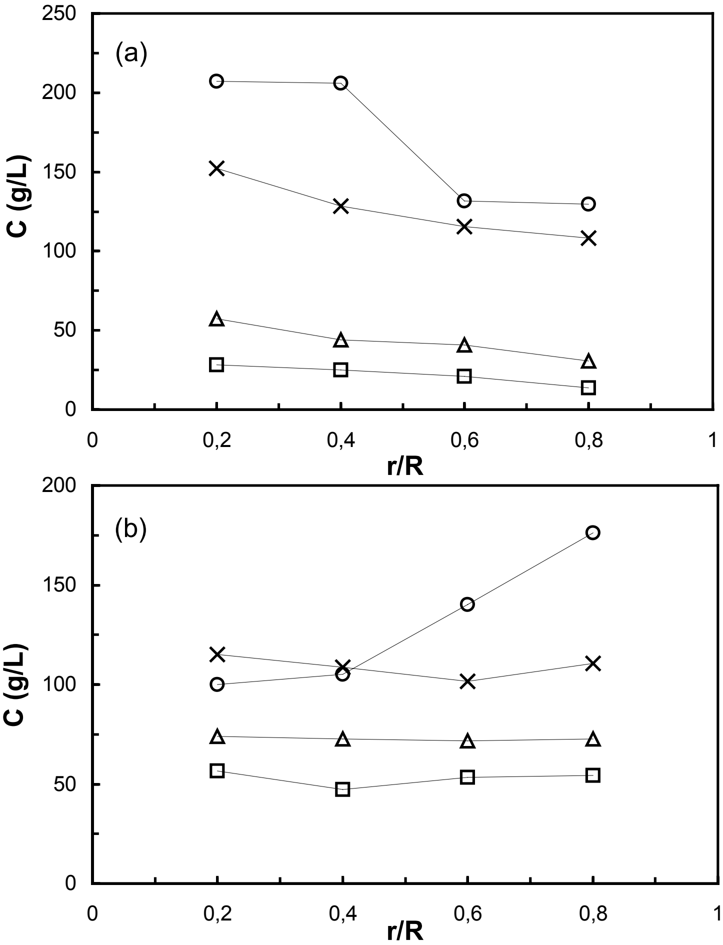

Figure 4 Radial solid concentration profiles at different elevations. (a) d_p=675 µm; (b) d_p=327 µm. (○) z=0.12m; (X) z=0.45m; (△) z=0.845m; (□) z=1.09m.

In Figure 5 the axial concentration profiles are shown as obtained by averaging the four concentration values at each elevation in the case of C_{av}=10 (d_p=327µm) and 15 g/L (d_p=675µm). It can be noticed that the biggest particles give rise to more inclined profiles, as was already found in previous work [6, 10]. Once the axial profiles pertaining to the average concentration 10 and 100 g/L (d_p=327µm) and 15 and 100 g/L (d_p=675µm) are normalised with the average integral concentration, the profiles are almost coincident for the same particle diameter, as is shown in Figure 6. This comparison suggests that for an average concentration of 0.4% to 4% by volume there are no significant interaction effects between the particles (Zisselmar and Molerus, 1979) – apart from a small difference below the lower impeller, where the particle concentration is maximum since it reaches about of 6 vol. %.

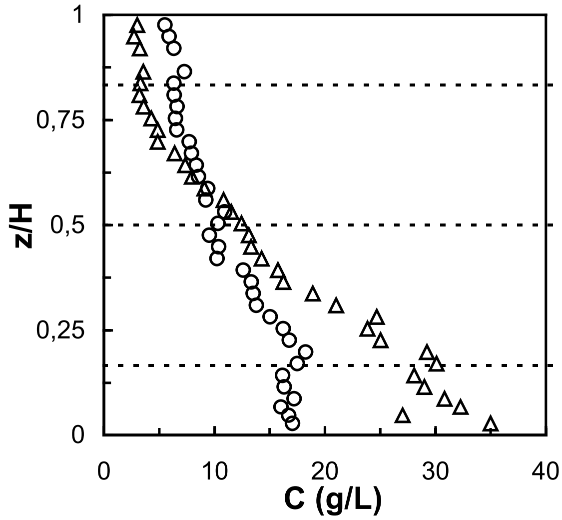

Figure 5 Axial solid concentration profiles.
(○) d_p=327 μm, C_{av}=10g/L; (Δ) d_p=675 μm, C_{av}=15g/L.

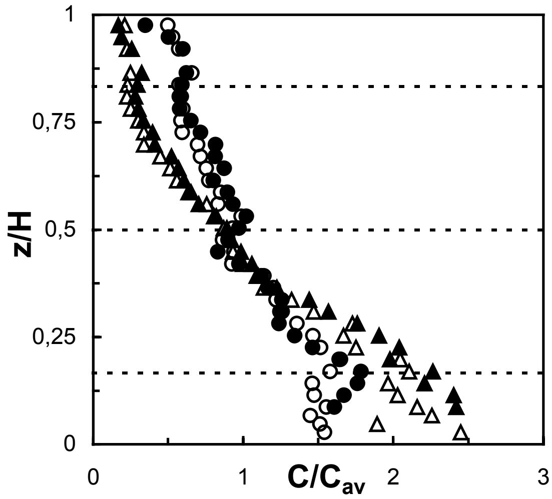

Figure 6 Comparison of normalised axial solid concentration profiles.
(○) d_p=327 μm, C_{av}=10g/L; (Δ) d_p=675 μm, C_{av}=15g/L; (●) d_p=327 μm, C_{av}=100g/L; (▲) d_p=675 μm, C_{av}=100g/L.

4.2 Liquid flow field predictions and comparison with literature experimental data

The fluid flow field significantly affects the solid distribution in solid-liquid stirred tanks, at least in the cases of dilute suspensions (Montante et al., 2001). Therefore, the validation of the simulated liquid flow field is an important step preliminary to the evaluation of the solid-liquid modelling. For this purpose, the predicted liquid flow field of the two-phase

simulations was compared with the LDV velocity data reported in (Kresta, 1992). The measurements were performed in a single-impeller, single-phase system. Because moderately dilute suspensions and highly spaced impellers are considered in this investigation, the comparison between these systems seems acceptable. In Figure 7 experimental and simulated axial, radial and tangential velocity profiles are reported along a radius underneath the impeller.
The simulation results were obtained by applying the MRF method and the Eulerian-Eulerian approach coupled with the Mixture turbulence model. As can be observed, the agreement between the experimental and the simulated data is fair; comparison at other elevations is satisfactory as well.
Also, the overall experimental pumping and power numbers were predicted with fair agreement. The power number, N_p, was calculated from the torque on the baffles and on the blades: both values were equal to 1.5 for each impeller and coincide with the experimental value measured in a single impeller system. The simulated pumping number, Fl, was equal to 0.8 when computed in the same way as the experimental data reported by Kresta (1992), who obtained the value 0.72 for the same impeller configuration.
The calculated slip velocity between the solid and the liquid were found to be very small, as was expected from previous experimental measurements (Nouri and Whitelaw, 1992; Montante and Lee, 1999).

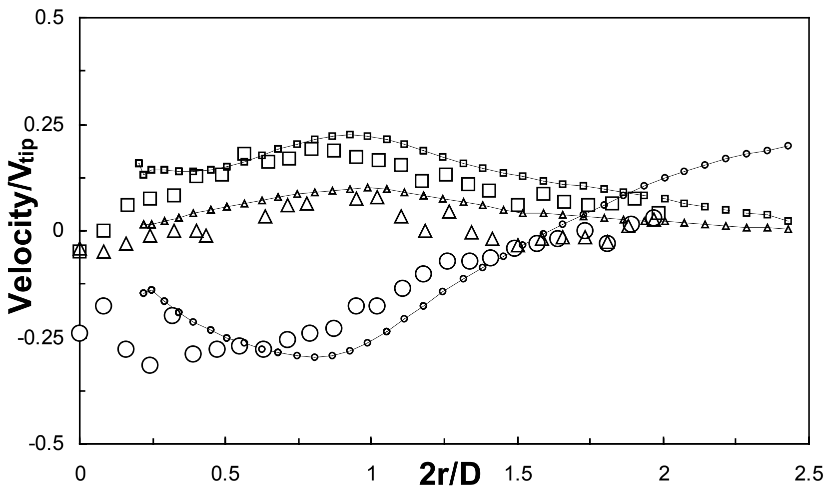

Figure 7 Comparison of LDV and CFD axial (○), radial (Δ) and tangential (□) velocity radial profiles on a plane at z/T=0.25 and mid-way between two baffles.

4.3 Solid particle distribution predictions and comparison with experimental data

After ascertaining that the solid-liquid modelling is reliable in representing the fluid flow field, a detailed analysis of the solid distribution predictions obtained with different combinations of two-phase and turbulence models was performed. The evaluation of the most suitable approach, in the case of the present solid-liquid system, is possible when comparing the simulated radial and axial solid concentration with the experimental data described above. The calculated solid distributions will be reported and discussed in the following sections.

4.3.1 Comparison of the results obtained with the Eulerian-Eulerian model coupled with three different two-phase turbulence models

The Eulerian-Eulerian model was adopted in conjunction with the available multiphase extensions of the k-ε turbulence model in order to identify which of them is more suitable to reproduce the solid distribution. The axial concentration profiles of d_p=327 µm particles and mean concentration C_{av}=100g/L are compared with the corresponding experimental data in Figure 8.

As can be observed, none of the simulated profiles is in agreement with the experimental data. Nevertheless, the comparison provides quite interesting information: the simplest 'mixture' turbulence model gives the same results as the more complex 'for each phase model' (they are practically coincident in the figure); both profiles show clear overestimation of the solid sedimentation in the lower part of the vessel. On the other hand, the 'dispersed' model, that in principle should be the most suitable for this solid-liquid case, provides a very strange trend, which is unjustified by the experimental data.

From this comparison it is possible to conclude that the Eulerian-Eulerian model as implemented in the commercial code is not accurate enough to catch the particle distribution in the tank, whichever turbulence model is adopted. However, among them, the simplest 'mixture' extension of the k-ε model seems to be preferred, at least for solid-liquid systems up to the present concentration of 4% by volume, as it provides the same quality of results as the most computationally expensive 'for each phase' model. This seems to suggest that for the concentrations considered in this work, no significant effect of the solid particle on the turbulent field of the liquid phase is present.

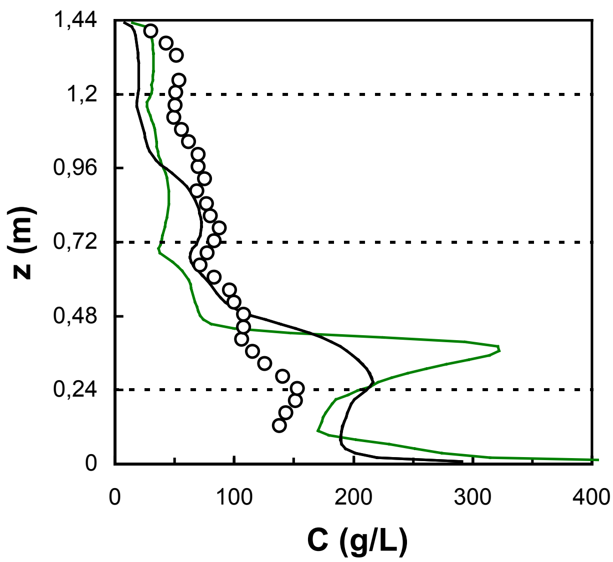

Figure 8 Comparison of the axial concentration profiles obtained with experimental data (O) and different turbulence models: (—) mixture; (---) for each phase; (—) dispersed.

4.3.2 Comparison of the Eulerian and the Granular modelling

In order to assess whether better spatial solid distribution could be obtained while taking into account the effect of the 'solid pressure' term in the two-phase model, Eqn (4), the experimental solid-liquid systems with the smaller and bigger particles were simulated with the Granular model, at the higher average concentration. The comparison of the simulated and experimental profiles is shown in Figure 9 (a),(b).

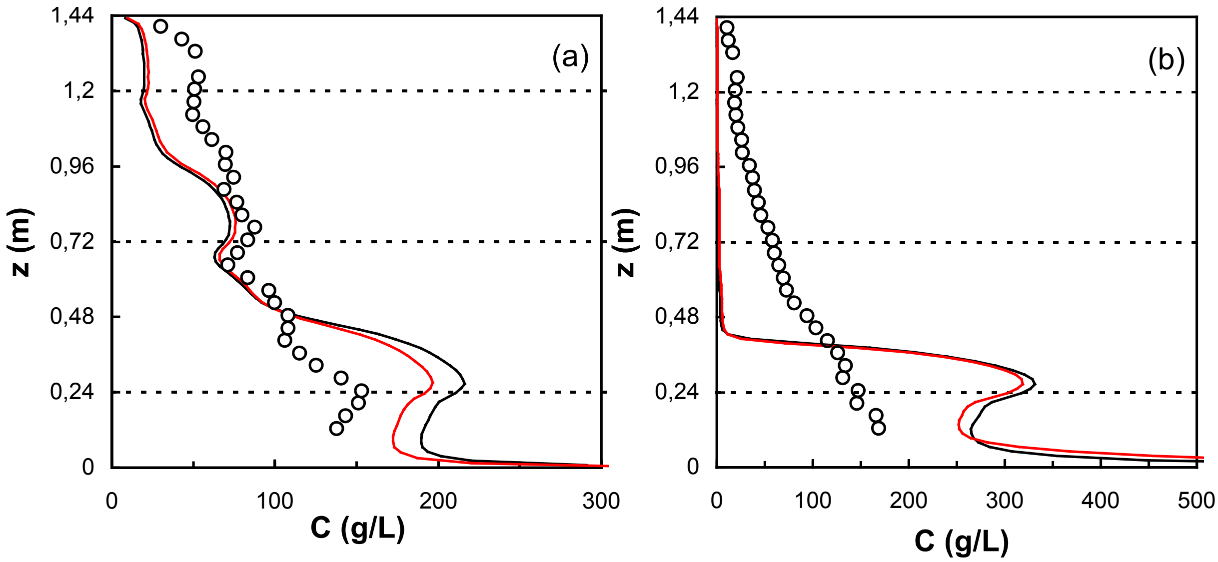

Figure 9 Comparison of the axial concentration profiles obtained with the Eulerian (—) and the Granular (—) models with experimental data (○). (a) d_p=327 μm; (b) d_p=675 μm.

Also the profiles obtained with the Eulerian-Eulerian approach coupled with the same turbulence model are reported in the figure for comparison purposes. For both the particle diameters, no discernible differences can be observed in the profiles obtained with the Eulerian and the Granular equations in the upper part of the vessel, where the concentration is lower. On the contrary, in the region of higher concentration, i.e. from the tank bottom to the region just above the lowest impeller, an improvement in the simulated profiles with respect to the Eulerian profile can be observed. However, the agreement with the experiment is still unsatisfactory and sedimentation is over-predicted for both the solid-liquid systems.

4.3.3 Effect of the particle drag coefficient on the solid particle distribution

It has already been shown in previous works (Micale et al. 200; Montante et al., 2001) that one of the most important parameters for the correct prediction of solid distribution in stirred tanks is the particle drag coefficient, C_D. In the commercial codes this parameter is usually estimated by means of the standard correlations valid for particles falling in a still fluid, while it has been experimentally observed that free stream turbulence may significantly modify the C_D value (Magelli et al., 1990; Brucato et al., 1998).
In the present work, overestimation of the solid concentration in the lower part of the vessel has been observed, with respect to the experimental data, with any of the tested multiphase models. This seems to suggest that the C_D value may be responsible for the observed discrepancy.
For this reason, the empirical correlation suggested in Pinelli et al. (2001) has been adopted in order to evaluate the effect of C_D on particle distribution. Figure 10 shows the results obtained for d_p=327μm, when the Eulerian-Eulerian Mixture model was applied with the value calculated from the mentioned correlation ($C_{D,turb}$=6.83).

As can be observed, the simulated profile is very different from that obtained with the same approaches and the standard $C_{D,still}$ value, and the agreement with the experiment is quite good.

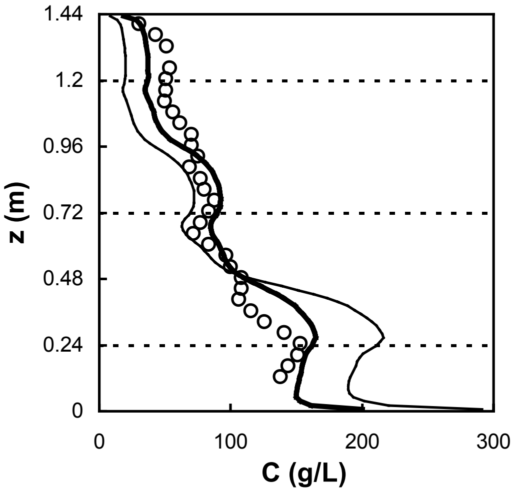

Figure 10 Comparison of the axial concentration profiles obtained with the Eulerian model and different correlation for C_D. (○) experimental data; (----) $C_{D,still}$; (▬▬) $C_{D,turb}$. d_p=327 µm.

The same result was obtained for the case of d_p=675 µm, whose profiles are reported in Figure 11.

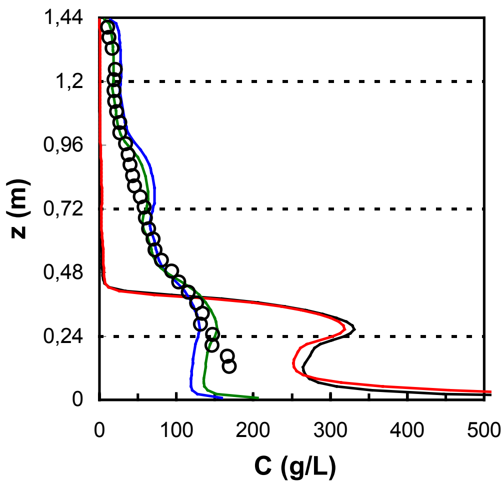

Figure 11 Comparison of axial concentration profiles obtained with different multiphase models and correlation for the C_D. d_p=675 µm. (○) experimental data; (—) E-E $C_{D,still}$; (—) E-E $C_{D,turb}$; (—) E-G $C_{D,still}$; (—) E-G $C_{D,turb}$.

Once again, the improvement of the results is apparent; notably, when the Granular model is applied in conjunction with the correlation given in Pinelli et al. (2001) the best agreement is found. A further test of the goodness of this approach is shown in Figure 12, where the comparison of simulated and experimental radial concentration profiles at different elevations is shown. As can be observed, also the predicted local concentration values are fairly close to the experiments.

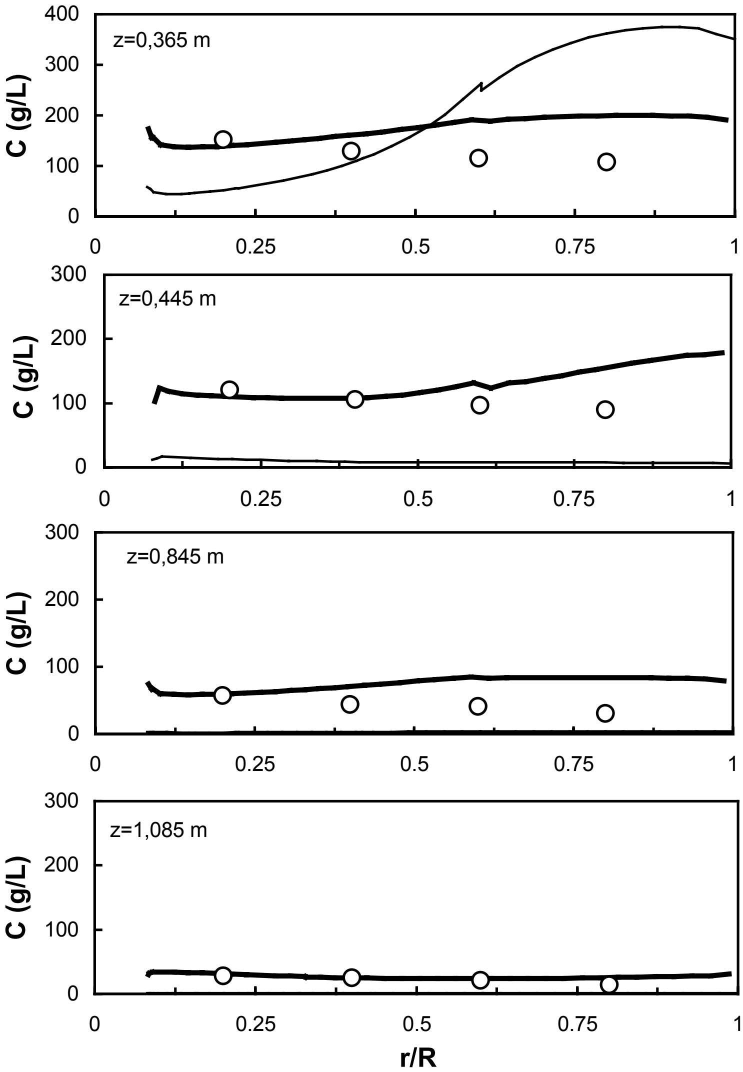

Figure 12 Granular simulation and experimental radial concentration profiles at different elevations. d_p=675μm, C_{av}=100g/L. (O) experimental data; (---) $C_{D,still}$=1.19 (Schiller & Naumann, 1933); (▬▬) $C_{D,turb}$=6.7 (Pinelli et al., 2001).

CONCLUSIONS

In this work, the solid concentration distribution of particles up to 4% by volume in a baffled, high-aspect-ratio tank agitated with three PBT was investigated by experimental measurements and CFD simulations. The simulation results were compared with the solid concentration data, obtained with a local optical technique, as well as with other literature data.

The CFD simulations were performed by adopting steady MRF fully predictive strategies for the baffled stirred tank and different multiphase and turbulence models implemented in the commercial CFD code Fluent 6.0.
As the solid distribution is greatly dependent on the liquid flow field, the CFD simulated velocities were first compared with literature velocity data and a fair agreement was found. Also, the predicted power and flow numbers were found to be in good agreement with the experimental data.
The Eulerian-Eulerian multiphase model was coupled with the available extensions of the k-ε model to the multiphase case, in order to investigate which of them was most appropriate to describe the solids distribution. The comparison between experimental and simulated solid concentration profiles has led to the conclusion that the 'mixture' model is the most proper among the turbulence models. It provides the same results as the more complex 'for each phase' model, while requiring less computational time and giving a qualitative fair representation of the solid distribution, whereas the 'dispersed' turbulence model gives rather unrealistic results.
The Granular modification of the Eulerian model for the solid phase provides an improvement of the predictions in the lower part of the vessel, where the highest particle concentration is present (up to 6 vol. %), with respect to the Eulerian model; while the same results can be observed in the rest of the tank where the solid concentration is lower.
It seems that the interaction phenomena between the solid and the liquid phases and those among the solid particles do not vary appreciably for solid concentrations up to about 4% by volume, while at higher concentration some effects become noticeable.
None of the models provides a fair representation of the solid distribution, unless a proper particle drag coefficient is adopted. The comparison between experiments and simulations clearly shows that a fundamental step to get reliable results is to implement a correlation that takes into account C_D modification due to the free stream turbulence effect.

ACKNOWLEDGEMENTS

This work was financially supported by the Italian Ministry of University and Research and the University of Bologna (PRIN 2002). The collaboration of Dr. D. Fajner, Mr. F. Orlandini and Ms. F. Bergonzoni in carrying out the experimental programme is gratefully acknowledged. This paper is based on the text of a communication accepted for presentation at the "8th International Conference on 'Multiphase Flow in Industrial Plants'" (Alba, September 2002), organised by ANIMP, Milano.

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