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Solid-Liquid Multiphase Flow Validation in Tall Stirred Vessels with Multiple Impeller Systems

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Abstract

The Eulerian-granular model as implemented in FLUENT 6 was validated based on experimental solids concentration data for a number of challenging validation cases consisting of tall stirred vessels equipped with multiple impellers. It was concluded that good results could be obtained for a variety of systems. The use of a correction to the standard drag laws for particles settling in still fluids is necessary to obtain good results in turbulent stirred vessels. Good results were obtained using eddy-viscosity turbulence models for fully baffled vessels. For unbaffled vessels, the use of the multiphase Reynolds stress model was necessary in order to obtain a good comparison between the experimental data and the predictions.

Introduction

Among the various industrial applications of stirred vessels, the agitation of solid-liquid systems is quite common. One important aspect of solid-liquid mixing is the distribution of solid particles inside the mixed volume, as in most cases it may affect the apparatus performance and the process efficiency. Over the years, novel experimental techniques for measuring the spatial solid distribution in solid-liquid systems have been developed and applied to collect information on a number of stirred vessel geometrical configurations of different scales and different solid-liquid systems by the Mixing Research Group at the Chemical Engineering Department of the University of Bologna.

Recently, FLUENT 6 has been used to predict the three-dimensional solid concentration distribution produced in a variety of mixing systems in the laboratory at Bologna. The aim was to determine a computational strategy that can be confidently applied to any stirred vessel and any solid-liquid system.

So far, CFD simulations of solid-liquid systems in stirred tanks published in the literature are concerned mostly with baffled vessels and single flat blade impellers. In this work, in order to demonstrate the reliability of the CFD procedure, particularly hard test cases were selected: all of them consisted of multiple impellers systems in tall vessels. These vessels are often adopted in industrial practice, but are more difficult to model than single impeller systems because exchange flows between the different circulation zones around the impellers have to be predicted correctly. Moreover, in multiple impellers tanks the axial profiles of solid concentration are often characterised by pronounced solid concentration gradients and singularities. These features are particularly suitable to point out any discrepancy between the simulations and experiments. Furthermore, unbaffled tanks have been considered, which are known to be much harder to model correctly because of the strongly swirling flow. The consistency of the simulation results with the actual behavior is demonstrated by comparing the FLUENT predictions with the experimental data.

Model Description

In the present work, the analyses were performed for tanks of different scales, both with and without baffles, agitated with different impellers: pitched blade turbines (PBT), standard Rushton turbines (RT), and Lightnin A310 hydrofoil impellers. Details about the systems studied are listed in Table 1. In all cases, experimental solid concentration data were available. These were collected with the optical technique used by Fajner et al. (1985) or by means of an optical probe (Montante et al., 2002). Impeller rotational speeds higher than the “just suspended” conditions were selected, to ensure that no solids were permanently settled on the vessel bottom. The flow was fully turbulent in all cases. A typical experimental system in the mixing laboratory at Bologna is shown in Figure 1.

The multiphase and turbulence models available in FLUENT 6, coupled with fully predictive impeller simulation strategies, have been tested in order to find out which of the different modeling techniques will lead to the most satisfactory representation of the flow field and solid distribution in solid-liquid stirred vessels.

A previous study (Montante et al, 2002) led to the conclusion that the Eulerian-granular model can be confidently selected. The lift force and the virtual mass force can usually be neglected in the calculations, as they give a minor contribution to the solution with respect to the other terms.

The inter-phase momentum transfer term is very important and it is modeled via the drag coefficient, C_D. In our experience, this last parameter is critically important for obtaining correct predictions of the solid distribution, thus special care has to be devoted to its choice. The drag correlations implemented in FLUENT 6 apply to particles falling in a still fluid. One of them has been tested in this work (Schiller and Nauman, 1935). It is well known that drag coefficients measured for single particles in still fluids do not necessarily apply to particles settling in a stirred turbulent fluid. Therefore, the effect of a correction to take into account the increase in the drag coefficient due to liquid turbulence was considered (Magelli et al., 1987 and 1990; Brucato et al., 1998; Pinelli et al., 2001).

According to Magelli and co-workers, the settling velocity for a particle falling in a stirred turbulent fluid, U_s, can be calculated from the settling velocity of the same particle in a still fluid, U_t, as follows:

$$U_s / U_t \ = \ 0.4 \left[\tanh \ (16 \frac{\lambda}{d_p} - 1) \ \right] + 0.6$$

Here d_p is the particle diameter and λ is the Kolmogorov microscale. The Magelli empirical correlation is very useful for evaluating the proper C_D value to adopt in the FLUENT simulations. The procedure used in this work was as follows. The terminal particle settling velocity U_t and corresponding drag coefficient were calculated using the Schiller-Naumann correlation. The average Kolmogorov microscale was calculated from the power input by the impellers. This then gave sufficient information to calculate U_s. Finally, the drag coefficient C_D that would result in U_s can be calculated from a force balance on the particles, which can be shown to result in the following simple relation:

$$C_D = C_{D,still} \left(\frac{U_t}{U_s} \right)^2$$

This constant C_D was then prescribed using a user-defined function (Fluent UDF Archive UDF52).

Finally, in order to close the problem, a suitable turbulence model has to be selected. Three different extensions of the standard k-ε model to multiphase systems are implemented in FLUENT 6. The simplest version, the "k-ε mixture model", was found to be accurate enough for the baffled tanks. As for the unbaffled vessels, a multiphase version of the Reynolds Stress Model has been recently developed (Cokljat et al., 2004) and it has to be adopted, as the two equations models fail to correctly predict the strong swirling flow in unbaffled systems. In all cases, the turbulent dispersion force in the momentum equations was enabled, which was found to be critical in order to obtain accurate results (by default this force is off in FLUENT 6).

For the baffled vessels, the model equations can be solved with the multiple reference frame (MRF) model, which allows simulating baffled stirred tanks at a relatively low cost compared to transient techniques such as the sliding mesh method. For the unbaffled cases, a single reference frame rotating with the impeller can be adopted. With respect to the numerics, we found that the flow in multiple impeller stirred vessels is sufficiently complex that numerical accuracy issues are important. All results reported here were obtained using unstructured hexahedral meshes in combination with higher order differencing schemes for both the momentum equations and the volume fraction. Ensuring full convergence of the results is also important. In addition to monitoring residuals, one needs to make sure that the physical variables themselves no longer change. It is recommended to monitor the volume averaged velocity magnitude and tangential velocity to ensure that the flow field is fully developed. Furthermore, local volume fractions should be monitored, either by means of point probes or by checking the axial concentration profile, to ensure that the results are fully converged.

Results

The capability of the selected computational strategy to closely reproduce the complex distribution of the solid particles in stirred vessels can be appreciated in the case of a baffled vessel stirred with three down pumping PBTs (Montante et al., 2002). In Figure 2, the axial profiles of solid concentration along the vessel height as predicted from the simulations are compared with the corresponding experimental data. The agreement between the experimental data and the simulation performed with the Magelli correlation (which resulted in a drag coefficient of $C_D = 6.7$) is essentially perfect, while the predictions using the Schiller-Nauman correlation are rather poor. The Schiller-Nauman correlation predicts too low a value for C_D, and as a result particles tend to settle more than what is observed experimentally.

What we learned during this project and our previous research (Montante et al., 2001 and 2004) is that in general, good results can be obtained only when Magelli's correlation is considered. It is important to keep in mind that in some cases, according to the correlation, the ratio U_s/U_t is close to one. In those cases, no correction to the standard C_D value is needed. Nevertheless, for each solid-liquid system, geometrical configuration, and operating condition one should calculate U_s/U_t before starting the CFD simulations in order to determine if the standard Schiller and Naumann drag law can be used, or if a modified drag coefficient should be used.

Two systems were studied for which $U_s /U_t \approx 1$ and for which we could therefore use the Schiller-Nauman drag correlation: a baffled and an unbaffled vessel with four Rushton turbines. The results for the baffled vessel with Rushton turbines are shown in Figure 2. The experimental profiles are closely followed by the simulation, even in the singularities that, for the RT case, appear above each impeller.

To get the same quality of result with unbaffled vessels was much harder. For unbaffled vessels, which exhibit strongly swirling flow, eddy-viscosity models will predict unphysical flow reversals and good flow field results can only be obtained using either a full Reynolds stress model or with large eddy simulation (Figure 4). Good results for the unbaffled Rushton system were obtained using the dispersed Reynolds stress model for multiphase flows. Figure 5 shows the local volume fraction in a cross section of the vessel. The poor mixing performance of this system is apparent. As a result of the segregated circulation patterns, most of the solids stay below the bottom impeller. The solids fraction near the upper impellers is much lower. Figure 6 shows a comparison between the experimental data and our model predictions. The normalized axial coordinate z/H is plotted on the y-axis, and the average solids concentration at that elevation is plotted on the x-axis. A good comparison is achieved, providing additional validation of the model.

The second unbaffled stirred tank validation involves the same vessel, but now equipped with four A310 hydrofoil impellers. This operating condition is not recommended by the impeller manufacturer (Lightnin), which recommends the use of baffles. However, experimentally it was observed that when this impeller is operated according to the manufacturer's recommendations, the solids concentration profile is relatively uniform. But when operated in an unbaffled vessel, a peculiar phenomenon is observed. The solids slowly move upwards through the vessel and accumulate in the top part of the vessel (Pinelli et al., 2001). This is a much more challenging validation case than the baffled operating condition, and hence we selected this more difficult case for our studies. For this system $U_s /U_t < 1$ and the Magelli correction had to be applied, which resulted in a drag coefficient $C_D = 5$. Figure 7 shows the local volume fraction in a cross section of the unbaffled vessel equipped with four A310 impellers using the dispersed RSM.

Simulations using the RNG k-ε model completely failed to capture this behavior. Figure 8 shows a comparison between the experimental data, the RNG k-ε results, and our current RSM predictions. The normalized axial coordinate z/H is plotted on the y-axis, and the average normalized solids concentration at that elevation is plotted on the x-axis.

It is obvious that the predictions using the RNG k-ε model do not match the experimental data at all. But a much better comparison is achieved between the RSM results and the experimental data, providing additional validation of the RSM. With RSM we are in fact able to also capture this rather peculiar behavior, with solids accumulating close to the vessel top.

Conclusions

We can conclude that FLUENT 6 can be confidently applied for predicting the solid distribution in solid-liquid stirred vessels using the Eulerian-granular model. Special attention has to be paid to the particle drag coefficient correlation. Indeed, the C_D is a critical parameter for the correct prediction of the solid distribution, and the use of the Magelli drag correction is recommended. Also the Reynolds stress turbulence model for multiphase flow is necessary for the case of unbaffled vessels, which are characterised by a strongly swirling flow. To obtain best numerical accuracy, the use of unstructured hexahedral meshes combined with second or higher order discretization schemes and deep convergence is recommended. Furthermore, the turbulent dispersion force in the momentum equations needs to be enabled which was also found to be critical in order to obtain accurate results.

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Symbols

C	Solids concentration (g/L)
C_{av}	Average solids concentration (g/L)
C_D	Drag coefficient (-)
$C_{D,still}$	Drag coefficient for a single particle falling in a still fluid (-)
d_p	Particle diameter (m)
D	Impeller diameter (m)
H	Vessel height (m)
T	Vessel diameter (m)
U_s	Particle settling velocity in a turbulent stirred vessel (m/s)
U_t	Particle settling velocity in a still fluid (m/s)
W	Impeller blade width (m)
z	Axial coordinate: vertical distance from the vessel bottom (m)
λ	Kolmogorov length scale (m)

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Table 1. Details of the systems studied.

Case	1	2	3	4
Impeller style	PBT (45°)	Rushton	Rushton	A310
Number of impellers	3	4	4	4
Baffles	4	4	0	0
Baffle Width (m)	0.048	0.0236	-	-
Vessel height (m)	1.44	0.944	0.944	0.944
Vessel diameter T (m)	0.48	0.236	0.236	0.236
Impeller diameter D (m)	0.195	0.0787	0.0787	0.0944
D/T	0.4	1/3	1/3	0.4
Impeller blade width W/D	0.28	0.2	0.2	-
Number of blades	4	6	6	3
Impeller Reynolds number	3.1E+05	1.0E+05	1.9E+04	1.7E+05
Impeller power number	1.5 (Exp.)	4.8 (Exp.)	2 (FLUENT)	0.2 (FLUENT)
Impeller spacing (m)	0.48	0.236	0.236	0.236
Lower impeller to bottom (m)	0.24	0.118	0.118	0.118
Liquid density (kg/m3)	997	997	997	997
Liquid viscosity (Pa-s)	0.001	0.001	0.0057	8.90E-04
Solid material	glass	glass	glass	glass
Solid density (kg/m3)	2450	2450	2450	2450
Solid particle diameter (mm)	0.675	0.137	0.327	0.327
Solid concentration (kg/m3)	100	1.67	2	1.3
Impeller RPM	484	975	1074	993
Computational mesh	Hexahedral	Hexahedral	Hexahedral	Hexahedral
Number of cells	117k	237k	80k	1100k
Section modeled (degrees)	90	180	60	120
Impeller model	MRF	MRF	MRF	MRF

Figure 1. A typical experimental set up in the mixing laboratory at Bologna.

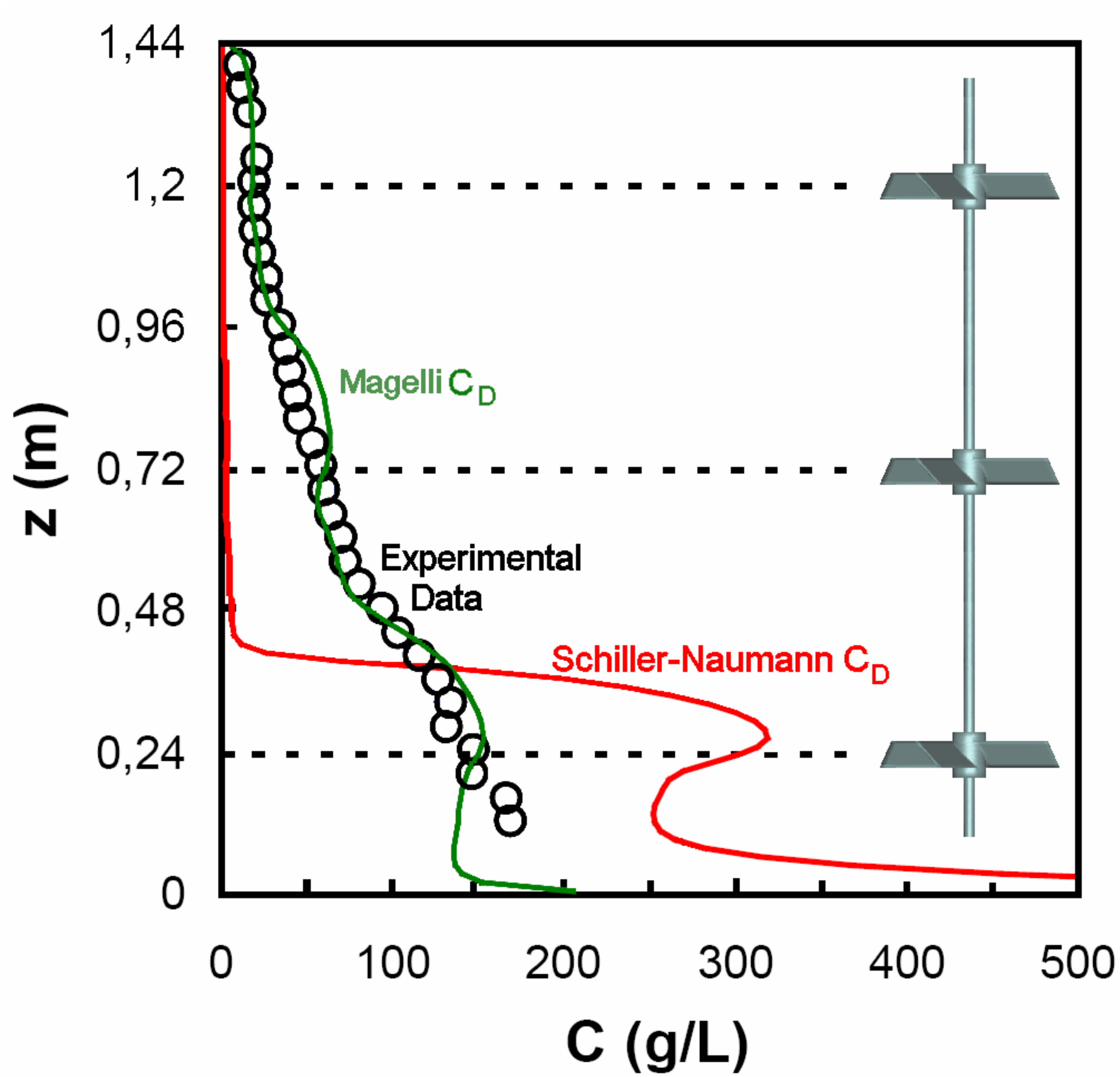

Figure 2. Baffled vessel equipped with three pitched-blade turbines. Solids concentration predicted by FLUENT 6 compared with experimental data using the Eulerian-Granular model for two different drag models. Glass particles with a diameter of 675 μm suspended in water. The solids concentration in the vessel C(g/L) is plotted on the x-axis, and related to the axial coordinate z(m) on the y-axis.

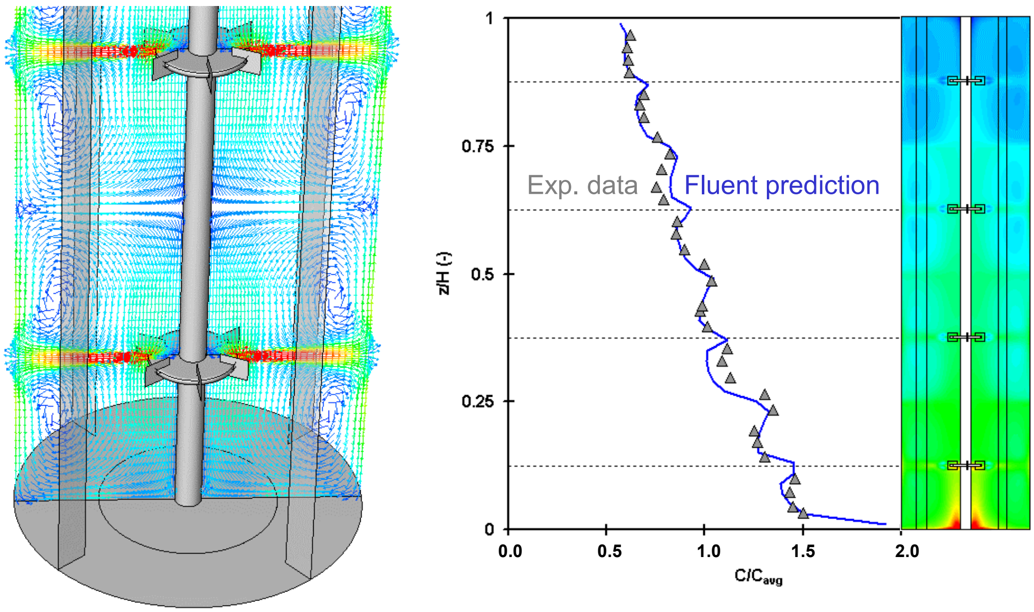

Figure 3. Flow field, solids volume fraction, and a comparison between the predicted solids volume fraction and experimental data for a tall baffled vessel equipped with four Rushton turbines.

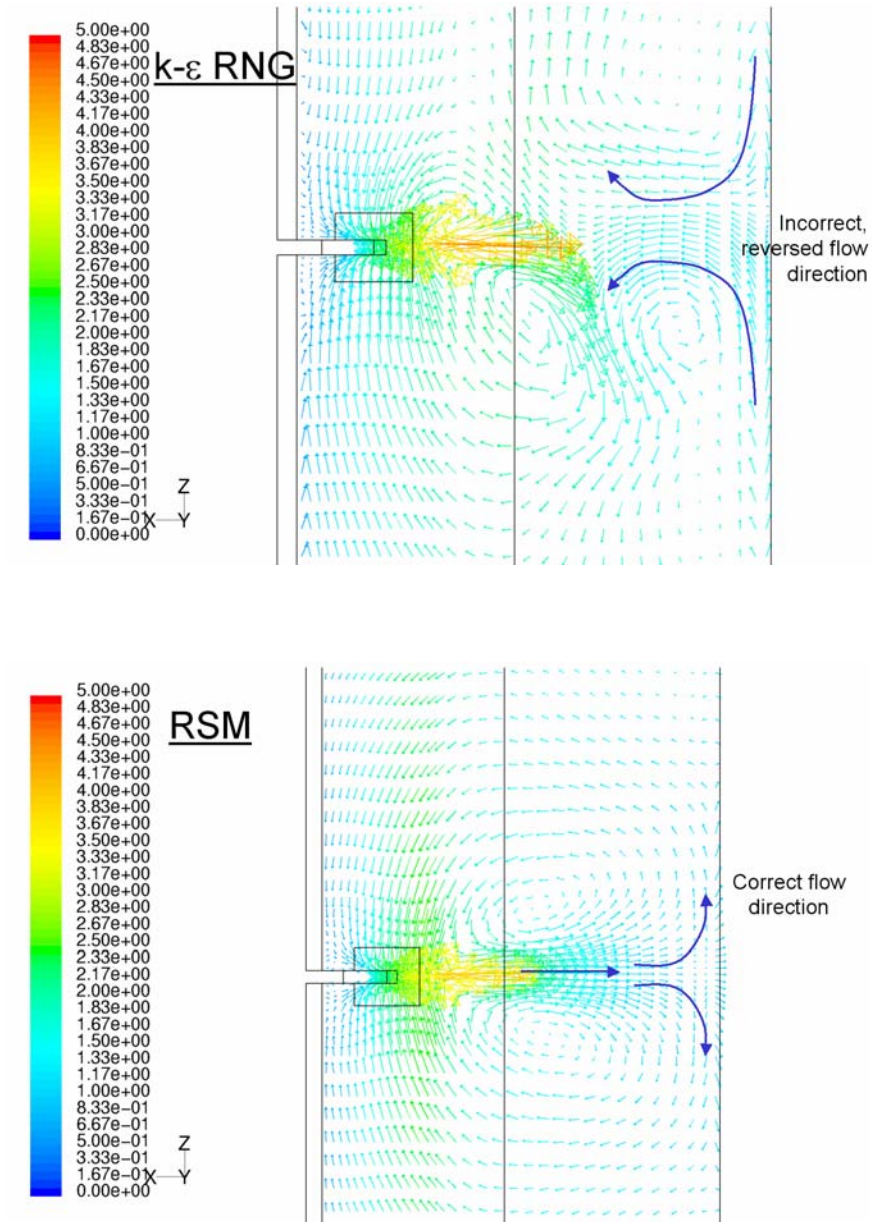

Figure 4. The flow in an unbaffled stirred tank equipped with a Rushton turbine is shown. The color indicates the velocity magnitude in m/s. When no baffles are present, the flow is dominated by a strong swirl. Strongly swirling turbulent flows are hard to model and most commonly used turbulence models will fail. The top picture shows the flow predicted by the RNG k-ε model. This model predicts an incorrect flow reversal near the impeller. All other so-called eddy viscosity models (k-ε, realizable k-ε, Spalart-Allmaras, k-ω) predict reversed, incorrect flow also. For swirling flows, only the Reynolds stress model (RSM; prediction shown on the bottom) and LES will predict the correct flow fields.

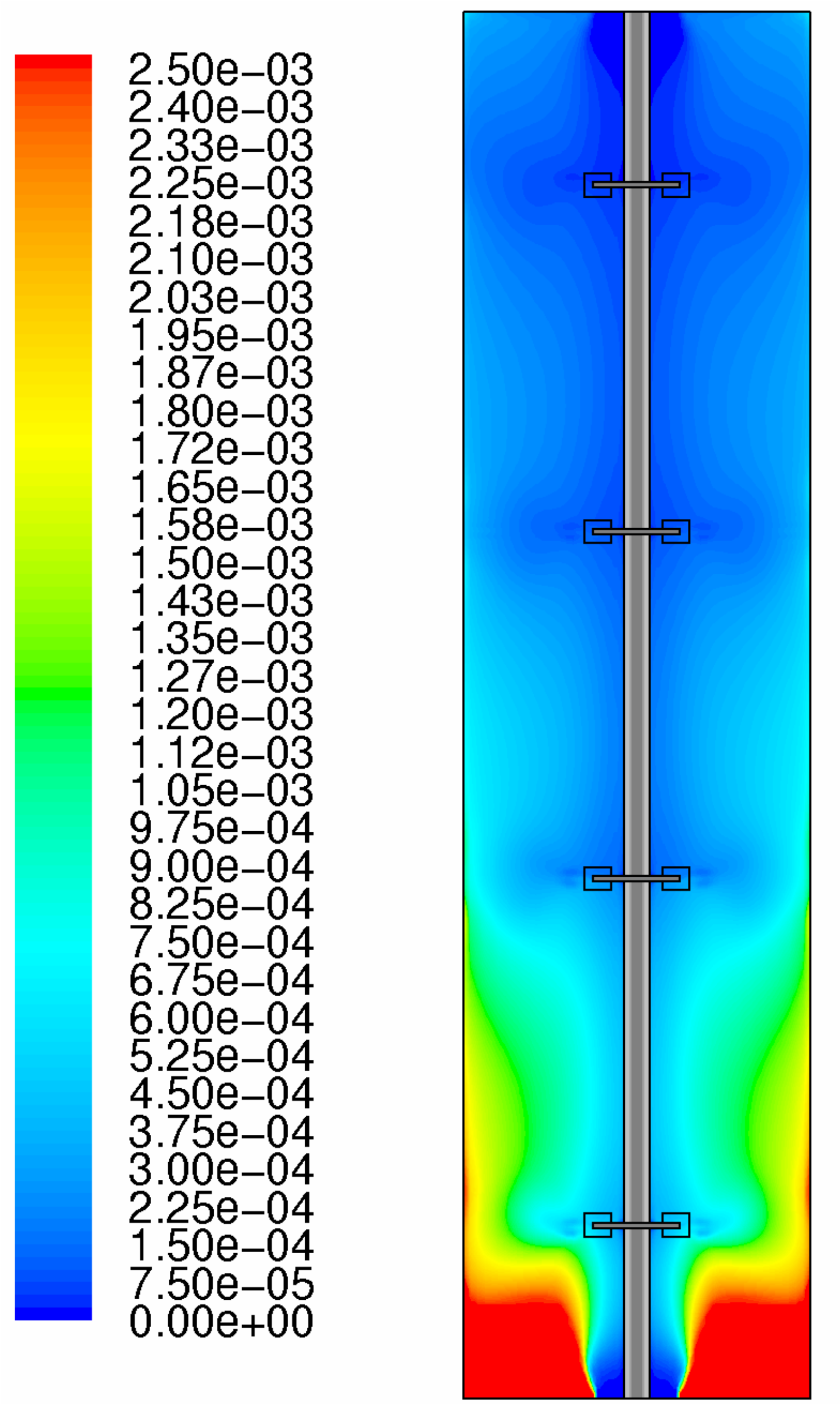

Figure 5. The local volume fraction of solids in a cross section of an unbaffled vessel equipped with four Rushton turbines, as predicted using the dispersed RSM.

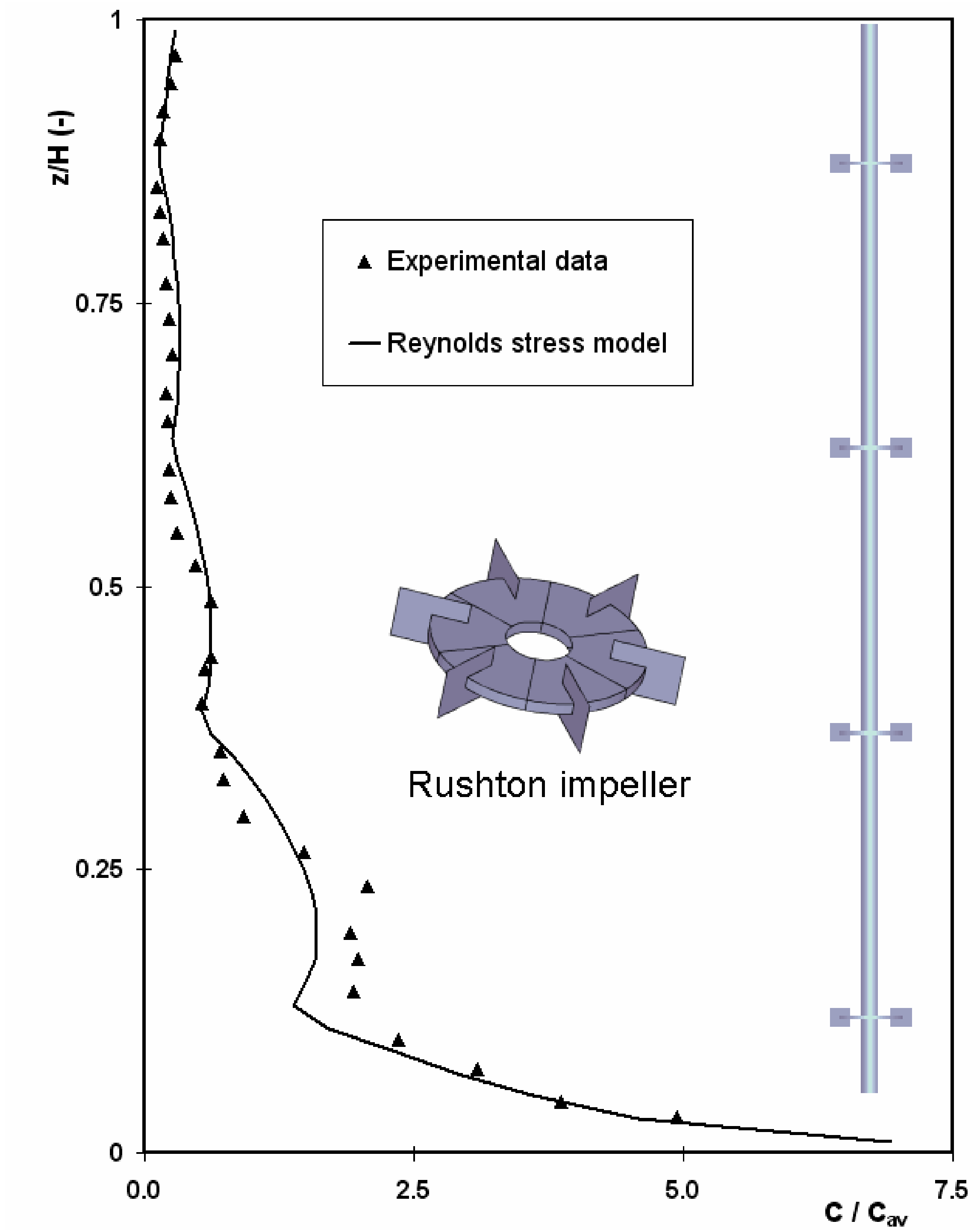

Figure 6. A comparison between experimental data from Pinelli et al., and predictions using the dispersed Reynolds stress model for an unbaffled stirred vessel equipped with four Rushton impellers. The normalized local solids concentration in the vessel C/C_{av} is plotted on the x-axis, and related to the normalized axial coordinate z/H on the y-axis.

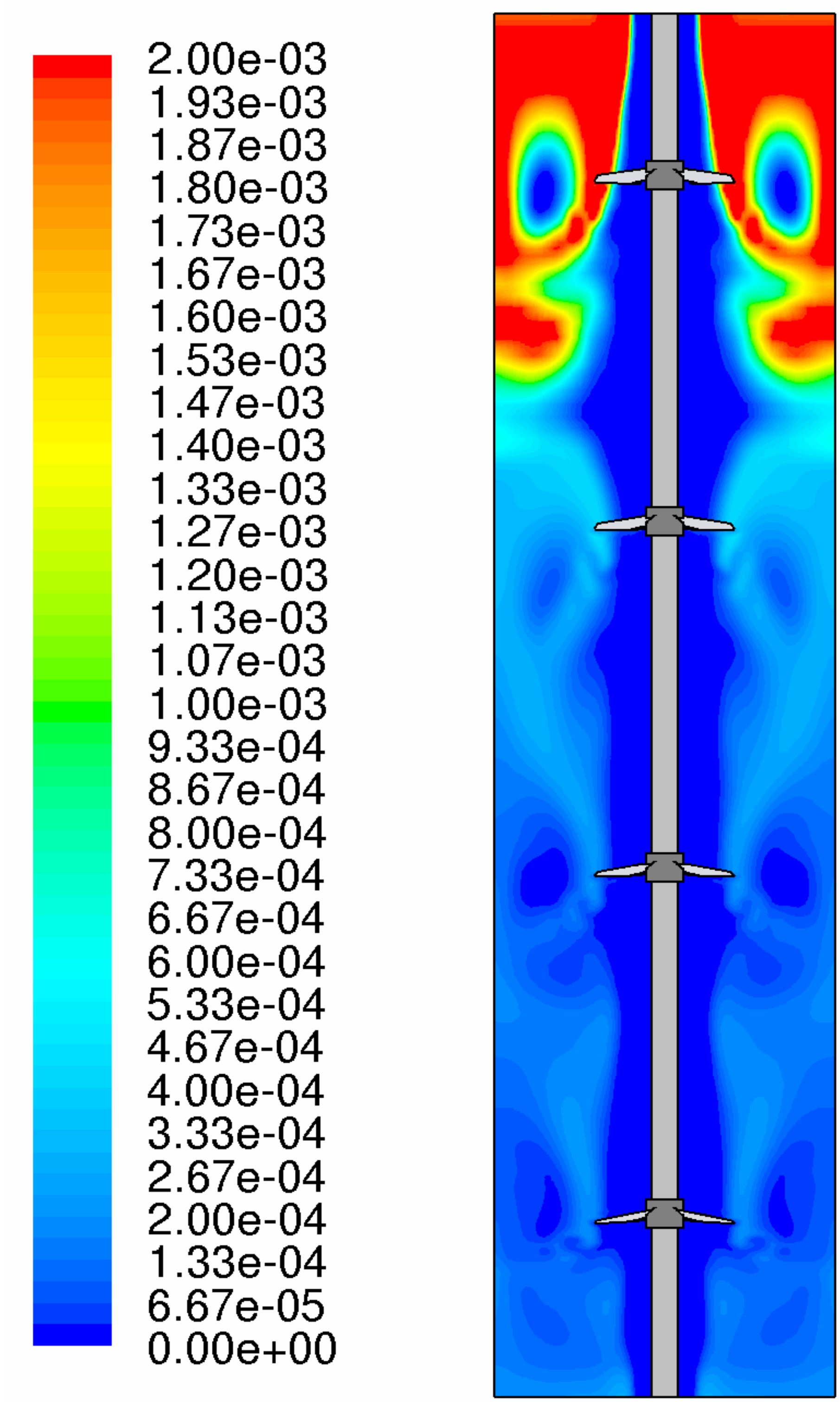

Figure 7. The local volume fraction of solids in a cross section of an unbaffled vessel equipped with four A310 impellers as predicted using the dispersed Reynolds stress model.

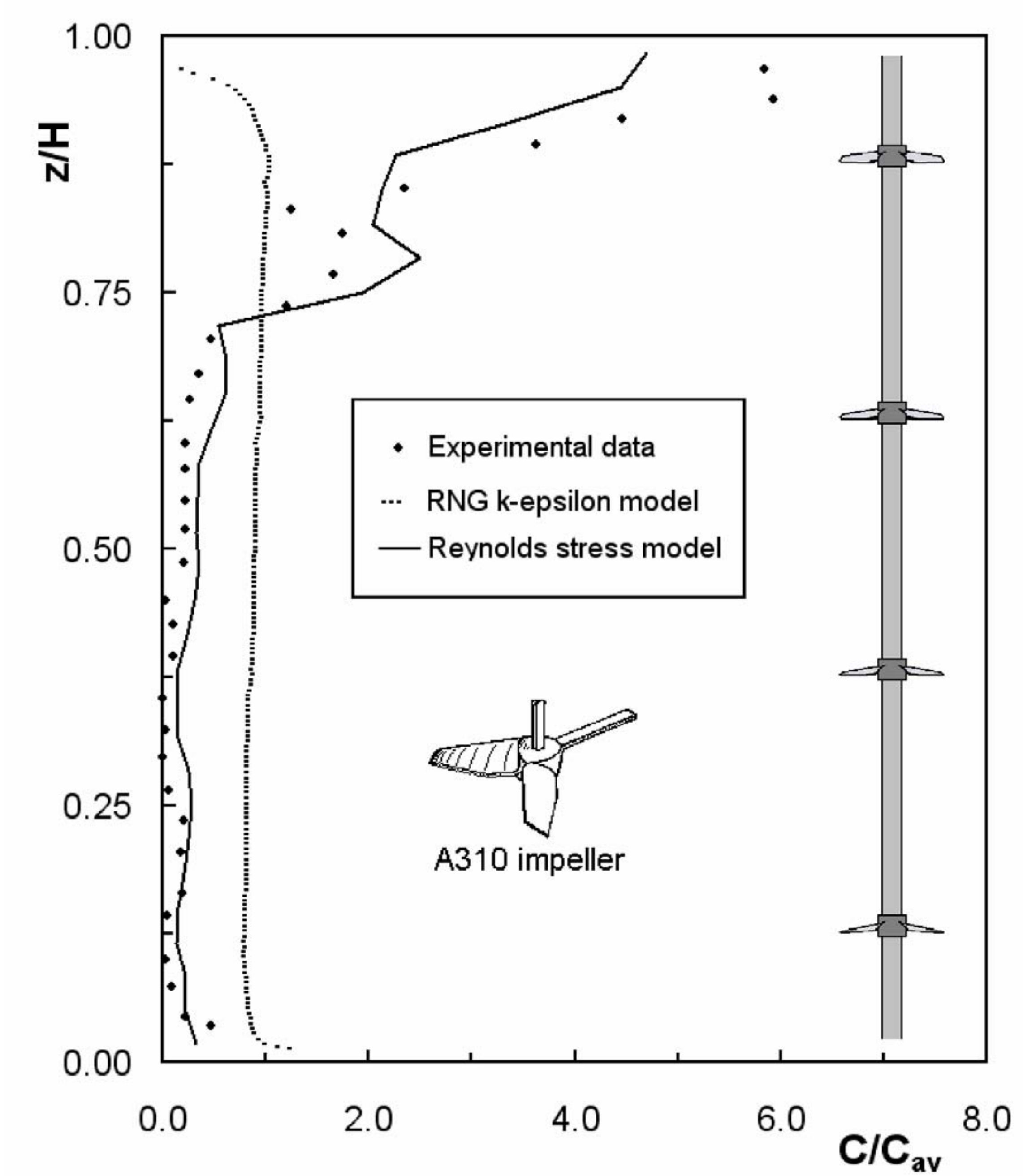

Figure 8. A comparison between experimental data from Pinelli et al., predictions using the RNG k-ε model, and the dispersed Reynolds stress model for an unbaffled stirred vessel equipped with four A310 impellers. The normalized local solids concentration in the vessel C/C_{av} is plotted on the x-axis, and related to the normalized axial coordinate z/H on the y-axis.