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Numerical Study of Stirred Tank with Multiphase System

Jiří Vondál*, Jiří Hájek, Miloslav Dohnal

Institute of Process and Environmental Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2, 616 69 Brno, Czech Republic
vondal@fme.vutbr.cz

The present work aims to develop a modelling approach for the simulation of multiphase stirred tank with floating particles, suitable for up-scaling studies. Multiphase numerical modeling is used for predicting velocity profiles in stirred liquid. Free surface is evaluated from gas-liquid phase interaction. Transient time is incorporated in simulation. Entire simulation is run in this mode. It includes impeller start-up phase from zero to the full speed. The methodology is demonstrated on a case of published stirred tank design previously analyzed by experimental methods. Scale-up of stirred tanks is a frequently faced problem, which is difficult in cases of multiphase systems, especially with floating particles. The methodology presented in this work is directly applicable in practical problems concerning the scale-up of such complex multiphase systems. Free surface effect on velocity profile and on drawn-down location of solids is presented. This is usually omitted and simplified as a flat surface.

1. Introduction

The body of scientific literature on the mixing of floating solid particles is relatively modest. Even though, several publications provide insights into the studied process, suitable tank, baffles and impeller design, as well as in computational modelling of such systems.

1.1 Drawdown mechanisms

Identification of mechanisms that can lead to drawdown of solids was studied by Khazam and Kresta (2009). They state that design requirements for this process are not completely defined, and are currently limited to heuristics regarding the use of a surface vortex and the effect of wettability on the difficulty of mixing, along with several initial studies in the literature. In their study, the effect of the type of impeller, particle size and shape, solids concentration, impeller submergence, and baffle configuration on the minimum drawdown speed are investigated. It was found that the formation of a large surface vortex acts to hold particles close to the surface. Suppression of the surface vortex is recommended. In baffled tanks where the formation of a large surface vortex is suppressed, the intensity of turbulence and mean circulation velocity of the liquid are responsible for solids drawdown and distribution in the tank. The submergence of the impeller relative to the liquid surface and the pumping mode of the pitched blade turbine were found to be the controlling parameters. CFD simulations were carried out to obtain a better understanding and interpretation of the flow patterns and drawdown mechanisms for the different baffle configurations. They conclude that only two mechanisms for solids drawdown are active in fully baffled tanks: mean drag and turbulent fluctuations.

1.2 Design of stirred tanks for draw-down of floating solids

Design options for solid drawdown in stirred tanks have been discussed by Khazam and Kresta (2009). Two mechanisms for the drawdown of floating solids in baffled stirred tanks have been identified: turbulent engulfment and mean drag. Baffling suppresses stable surface vortex formation and increases the intensity of mean drag and turbulence at the surface. Strong top to bottom liquid circulation is also promoted by baffling, however; this circulation rapidly brings particles back to the surface. In this paper, two alternate baffle configurations are proposed: half baffles and surface baffles. The objective is to maintain a high level of turbulence at the surface while reducing the return circulation from the bottom of the tank. It is found that half baffles are very similar to full baffles in performance, but surface baffles offer

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several advantages: a significant reduction in just drawn down speed, more robust performance at large submergences, and a better distribution of solids.

General guidelines regarding the design of baffles that optimize mixing characteristics are provided by Myers et al. (2002). The authors conclude that when agitating low-viscosity liquids, standard baffling typically provides near-optimal process performance and good mechanical stability. In addition, standard baffling is backed up by extensive design and scale-up data. The observations presented by the authors are intended to identify baffle system modifications that can be used to improve performance and the situations in which these modifications should be considered.

1.3 Scale-up criteria

The effect of scale on drawdown of floating solids has been studied in an experimental analysis (Özcan-Taşkin, 2006) that addressed the importance of impeller type, pumping mode and position, plus the effect of varying liquid height. Results from different scales are discussed in relation to the way in which solids are drawn down from the liquid surface. The study shows that over a wide range of conditions the power required for drawing down solids can be reduced by operating in the upward rather than downward pumping mode and using an axial flow narrow blade hydrofoil rather than a mixed flow pitched blade turbine. Different scale up criteria, power per unit volume, tip speed and Froude number, are discussed for these systems. For scale up, specific power input is shown to be the most appropriate criterion for upward pumping impellers.

Contrasting with the latter publication are results of Waghmare et al. (2011). This work shows development of a scale up correlation using computational fluid dynamic (CFD) simulations for floating solids drawdown operation in stirred tanks. Discrete phase modelling (DPM) simulations were used in conjunction with the lab scale experimental measurements to develop a semi-empirical correlation for the prediction of rate of drawdown of floating solid particles. The rate was correlated to average liquid velocity at the free liquid surface. Since, this correlation is based on a fundamental hydrodynamic parameter, velocity, rather than an operating parameters such as the impeller speed, it can be used for a variety of impeller types and tank geometries. The correlation was developed based on the data obtained from the 0.002 m^3 tank using four different tank designs and was validated against the data obtained from the 0.010 m^3 scale tank. The correlation was further extended to the pilot and the commercial scale tanks ranging from 0.040 m^3 to 4 m^3 scale based solely on the CFD model.

The third work dealing with scale-up of stirred tanks comes from the Czech Technical University in Prague (Svačina, 2013). Linear dependence of just draw down rotation speed on floating solids concentration was verified. From all investigated configuration, the lowest impeller rotation speed needed for particle drawdown in a fully baffled vessel is achieved by upward pumping impeller placed near to a liquid surface. This configuration also requires the lowest power per volume (specific power input). The most energetically demanding configuration is downward pumping impeller placed near to a vessel bottom. On the other hand, this configuration proves the best redistribution of submerged particles in the vessel volume. For scale-up, constant tip speed was found to be the best appropriate criterion to model scaling of standard 45° pitched four-blade turbine downward pumping impeller (4-PBT-45°) placed near to a bottom in a fully baffled tank. For downward pumping impeller placed near to a liquid surface, criterion of constant power per unit volume correlates this geometry the best. In case of upward pumping impeller, the factor of impeller submergence seems does not play an important role.

After analysis of literature sources that provide recommendations for the use of scale-up criteria, it has been concluded that probably the best criterion available is the one proposed by Waghmare et al. (2011). It seems to be quite general with respect to impeller design and is based on data from both experiment and simulations, which makes it suitable for use in computational studies. The other criteria found in the literature are mostly less general. Moreover, most of the published scale-up criteria have been developed for up-pumping mode, which is reportedly less energy-demanding for the same drawdown rate of floating particle.

1.4 Modelling of stirred tanks with floating solids

The modelling of stirred tanks with solid particles (both floating and settling) is possible in a number of ways, using a wide range of models as discussed in the review paper of Ochieng and Onyango (2010). For solid–liquid mixing, traditionally the research efforts were geared towards determining mixing features such as off-bottom solid suspension using experimental techniques. The 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 modelling 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.

Useful information about suitable modelling approaches can be extracted from several works. Özcan-Taşkin and Wei (2003) performed a comparative analysis of velocity profiles predicted in a 90° periodic slice of the stirred tank by CFD and measured by laser Doppler anemometry. The intensity of draw-down was however compared only by visual observations. Two baffle configurations were investigated by Khazam and Kresta (2009) by experiments and CFD modelling, although using major model simplifications including flat liquid surface and steady-state approach. To describe impeller movement, they used multiple-reference frame (MRF) approach, which is a steady-state simplification of the stirring, where actual impeller rotation is modelled by source terms in the impeller volume. An Euler-Euler approach to modelling of the dispersed phase in liquid was used by Mohanarangam and Stephens (2009), together with an algebraic slip model. Authors of the work studied both floating and settling solids, but the tank was not stirred. Unbaffled tanks were investigated with a MRF CFD model by Ciofalo et al. (1996), in this work without any dispersed phase particles. A CFD modelling methodology for sedimentation has been reported by Tarpagkou and Pantokratoras (2013) with Lagrangian description of the secondary particulate phase and two-way coupling between the two phases.

Waghmare et al. (2011) reported a unique scale-up study performed using computational fluid dynamics (CFD) modelling combined with experiments in the small scale. The CFD simulations are performed using MRF approach. The authors chose to use this simple methodology due to much higher computational costs of a more precise unsteady sliding-mesh approach. Furthermore, they assumed the surface is flat and neglected sloshing of the real free surface. However, they included the floating solids by means of a Lagrangian discrete phase model.

2. CFD modelling approach

The present work introduces a novel advanced methodology for the modelling of stirred tanks with floating solids, which extends the capabilities of CFD models previously reported in the literature, such as Zhang et al. (2013). The methodology is designed with the purpose of quantitatively assessing the intensity of draw-down of floating solid particles. For the modelling was used commercially available code ANSYS FLUENT v.15.

2.1 Stirred tank set-up

The stirred tank used for a demonstration of the proposed methodology is adopted from Özcan-Taskin and McGrath (2001). That work reported experimental results (no simulations), but provided a complete specification of the mixed vessel including the impeller and baffles.

The stirred tank used in the present work is a laboratory-scale reactor with diameter of 0.310 m and the same liquid height. The reactor has a torispherical base and the same torispherical cap was used in the simulations to close the top of the vessel, with the quiescent liquid level at 2/3 of the total reactor height. The liquid volume is 0.0217 m^3.

Impeller used in the simulation is a mixed flow pitched blade turbine with four blades inclined at 45°. Its diameter is 0.104 m and it was used in a down-pumping mode. The impeller was submerged by 3/4 of the liquid height (bottom clearance 1/4 of liquid height). Operating conditions selected for the simulation are characterized by impeller rotation speed of 440 rpm, which was chosen at the higher limit of values in (Özcan-Taskin and McGrath, 2001).

Created numerical grid consists of 800,000 cells. 113,000 cells are hexahedral and the rest are tetrahedral.

2.2 Modelling methodology

The modelling methodology adopted in this work has been devised in such a way so that it enhances the previously reported modelling reported in the literature, as summarized in the chapter 1.4. First and foremost, the simulation is transient, in order to precisely account for the movement of impeller. The rotation of impeller is thus modelled directly, using a so-called sliding mesh approach. Whole reactor geometry is simulated to avoid enforced rotational periodicity.

The deformations of liquid surface were also taken into account by means of a volume-of-fluid (VOF) approach. This approach enables to precisely predict velocity distribution in the liquid near the surface level, which is important for the draw-down of floating particles. In order to precisely predict a sharp interface between liquid and gas, a coupled level-set and VOF model was used. This approach is a suitable option for two-phase flows with topologically complex interfaces, as it provides both volume conservation and accurate estimates of interface curvature and surface tension force caused by the curvature. Volume fraction was discretized in time by explicit scheme and the face fluxes have been interpolated using interface reconstruction.

Momentum transport equations were discretized by second-order differencing as well as the transient terms in all governing equations. Pressure-velocity coupling was performed using the SIMPLEC scheme (Patankar, 1980). Turbulence was modelled by invoking the Boussinesq hypothesis, using a two-equation model, specifically the so-called realizable *k-ε* model (Shih et al., 1995). Unsteady solver was adopted with time step set to 0.0008 s.

3. Scale-up methodology

The scale-up criterion selected as a basis for the design of the present modelling methodology based on Waghmare et al. (2011) has quite clear physical explanation. It is based on the premise that the main mechanism for drawdown of the floating particles is mean drag, which is related to the average velocity magnitude on the liquid surface. Mean drag is a function of slip velocity between the solid particle and the liquid phase. These ideas lead to the conclusion that particle drawdown rate is governed by the velocity at the free liquid surface, as demonstrated by Waghmare et al. (2011). The concept of mean drag further suggests that the particle residence time on the surface is governed by the tank diameter, as in case of larger tanks particle has to travel greater distance to reach the wall before getting pulled into the liquid.

There are only two situations, where the surface-velocity scale-up correlation is not suitable. First is the case of strongly vortexing flows such as in unbaffled tanks. Second is the case of flows with strongly distorted free surface. The present case shows that there is mild distortion on the liquid surface, but the central vortex is not present due to baffles as shown in Figure 1. Also the impeller is deeply submerged and does not interact directly with the fluid surface. Therefore it seems that the correlation is suitable for the present process.

Further advantage of the selected scale-up methodology is that discrete phase modelling is not necessary. The model for discrete particles to take into account all relevant physics (wettability, clustering and effects of surface tension) would require large computing efforts and advanced modelling on the outer fringes of current state of the art. These efforts can be safely omitted, as long as a laboratory-scale data for the specific liquid, particles and gas are available. The scale-up correlation employs a single proportionality parameter that is easily determined from the laboratory data. CFD then may be used to optimize the up-scaled stirred tank and impeller at reasonable CPU costs.

4. Results

From a start-up condition with zero velocity inside whole tank to the full operation was 3 seconds in physical time. Within simulation it took about 3750 time steps to reach stable operation mode and developed flow patterns. On 8-core processor it took 3 d of computations.

In stable mode there are created two recirculation zones. The first can be clearly seen in Figure 1 forming next to the baffles. The second zone is formed under the impeller with only local significance. The primary recirculation zone is responsible for draw down of solid floating on the free surface.

From both Figures 1 and 2 can be seen that the free surface is mildly deformed. In those figures the surface is created as an iso-surface where the volume fraction of the gas is zero. It is in quasi-steady mode without visible influence of the impeller blades. With neglecting of such a deformation there may be employed significant error in simulation. We therefore encourage using free surface in simulations whenever possible.

Locations where the particle drawdown occurs are highlighted in Figure 2 by streamlines released from the surface. One location is next to the baffles while the other is next to the shaft.

The average velocity magnitude at the free surface is 0.184 m/s. The information about average surface velocity is not able to represent subtler changes in the character of flow. It is therefore advantageous to provide a surface velocity histogram, which may provide more insight, see Figure 3.

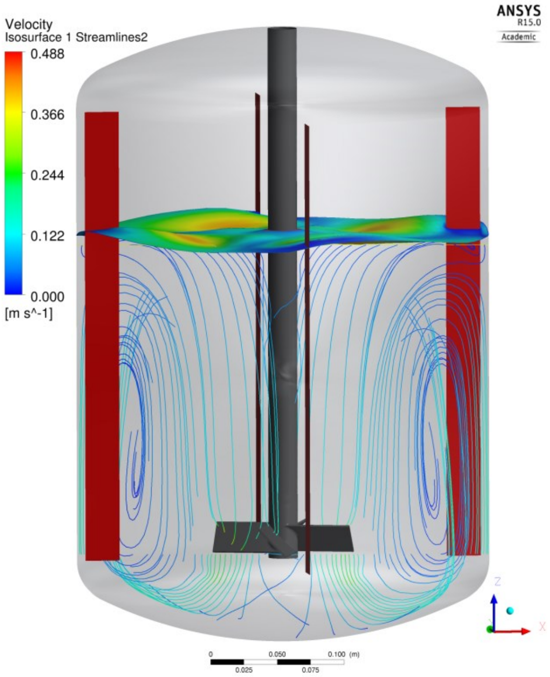

Figure 1: Recirculation zone marked by streamlines

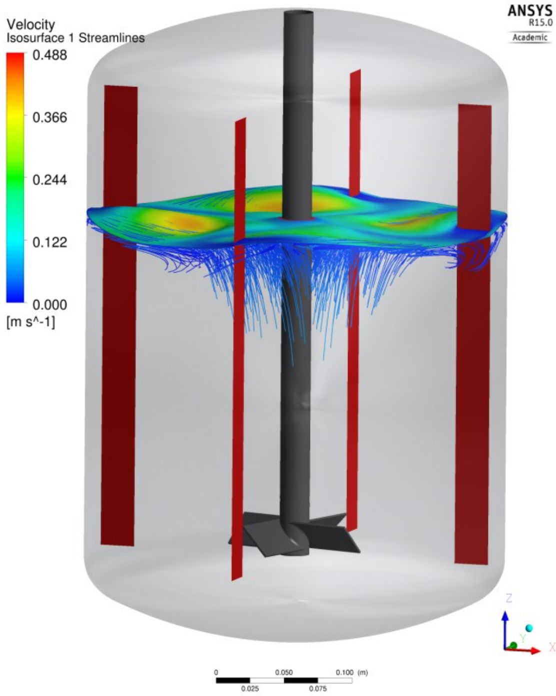

Figure 2: Drawdown location visualised by streamlines

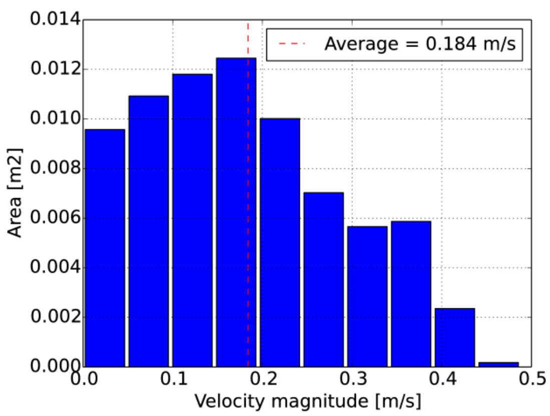

Figure 3: Histogram of velocity magnitudes on the free surface

5. Conclusions

The conclusions of the present work may be summarized as follows:

- Based on a literature review, suitable criterion for CFD-based scale-up was identified.
- Methodology for CFD simulations of stirred tanks with floating particles has been described, compatible with the scale-up criterion.
- Velocity and deformation of the free surface were shown for specific RPM based on experimental just-drawn-down speed.
- Locations where particles are drawn down were described.

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References

Ciofalo M., Brucato A., Grisafi F., Torraca N., 1996, Turbulent flow in closed and free-surface unbaffled tanks stirred by radial impellers, Chemical Engineering Science, 51(14), 3557–3573.

Khazam O., Kresta S. M., 2009, A novel geometry for solids drawdown in stirred tanks, Chemical Engineering Research and Design, 87(3), 280–290.

Mohanarangam K., Stephens D.W., 2009, CFD modelling of floating and settling phases in settling tanks, CSIRO, Melbourne, Australia. <www.cfd.com.au/cfd_conf09/PDFs/214MOH.pdf> accessed 2011/2013

Myers K. J., Reeder M. F., Fasano J. B., 2002, Optimize Mixing by Selecting the Proper Baffles, CEP magazine, 42–47.

Ochieng A., Onyango M., 2010, CFD simulation of solids suspension in stirred tanks: Review, Hemijska industrija, 64(5), 365–374.

Özcan-Taşkin G., 2006, Effect of scale on the draw down of floating solids, Chemical Engineering Science, 61(9), 2871–2879.

Özcan-Taskin G., McGrath G., 2001, Draw Down of Light Particles in Stirred Tanks, Chemical Engineering Research and Design, 79(7), 789–794.

Özcan-Taşkin G., Wei H., 2003, The effect of impeller-to-tank diameter ratio on draw down of solids, Chemical Engineering Science, 58(10), 2011–2022.

Patankar S. V., 1980, Numerical heat transfer and fluid flow, Hemisphere Pub. Corp. ; McGraw-Hill, Washington; New York.

Shih T.-H., Liou W. W., Shabbir A., Yang Z., Zhu J., 1995, A new k-[epsilon] eddy viscosity model for high reynolds number turbulent flows, Computers & Fluids, 24(3), 227–238.

Svačina O., 2013, Scale-up of stirred tank with floating particles, Faculty of Mechanical Engineering, Czech Technical University in Prague. <chps.fsid.cvut.cz/pt/2013/pdf/3510.pdf> accessed 26.02.2015

Tarpagkou R., Pantokratoras A., 2013, CFD methodology for sedimentation tanks: The effect of secondary phase on fluid phase using DPM coupled calculations, Applied Mathematical Modelling, 37(5), 3478–3494.

Waghmare Y., Falk R., Graham L., Koganti V., 2011, Drawdown of floating solids in stirred tanks: Scale-up study using CFD modeling, International Journal of Pharmaceutics, 418(2), 243–253.

Zhang S., Müller D., Arellano-Garcia H., Wozny G., 2013, CFD Simulation of the fluid hydrodynamics in a continuous stirred-tank reactor, Chemical Engineering Transactions, 32, 1441-1446, DOI: 10.3303/CET1332241