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Simulation of Multiphase Flow in Stirred Tank of Nonstandard Design

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Stirred tanks are commonly utilized in food, pharmaceutical and chemical industries. Most engineering applications make use of more or less standard design of a tank based on typical dimensions and shapes of key parts of the tank, which include diameter and shape of the stirred vessel, number, type and diameter of impellers and number, dimensions and shape of baffles.
The present work deals with a nonstandard stirred tank in terms of the geometrical configuration. The tank is used in pharmaceutical industry for processing eggshells. Computational Fluid Dynamics is employed to analyse flow conditions in the stirred tank during a batch process. Volume of fluid model is used to predict generation of the central vortex. Effects of various baffling (number and pitch angles) on the predicted flow field and central vortex shape are studied. All simulations are performed under typical operational conditions of the process such as an impeller speed and water volume.

1. Introduction

Stirred tanks are commonly utilized in food, pharmaceutical and chemical industries. Their main purpose is volumetric homogenization and intensification of processes such as heat and mass transfer. Characteristic feature of many stirred tank applications is multiphase flow, e.g. mixing of solid particles immersed in a liquid.

1.1 Standard design of a stirred tank

Stirred tanks have been given much attention both in experimental and theoretical studies. Research works provide valuable information on complex flow patterns and important engineering parameters for a standard design of stirred tanks. These include mechanical power of an impeller shaft, pumping volumetric flow rate and geometrical configuration of key components such as diameter and shape of the stirred vessel, number, type, position, diameter and rotational speed of impellers and number, dimensions, position and shape of baffles.
The key components together with physical properties of both solid and fluid (e.g. viscosity, density, particle mass loading) are major factors that establish flow pattern in the vessel (Kumaresan et al., 2006). Depending on a specific application, baffling is not necessary, but it is typically used to disrupt tangential flow. An insertion of the appropriate number of baffles significantly enhances mixing in the entire volume of the vessel (Myers et al., 2002). However, an excessive baffling may, under certain conditions, interrupt liquid mixing and prolong mixing times (Lu et al., 1997).
Effects of impeller types on flow pattern and process parameters including energy efficiency are studied as frequently as that of baffling. For instance, Molnár et al. (2013) investigated effects of various numbers of Rushtone turbine blades on homogeneity of the mixture and electrical power consumption. The Rushtone turbine is used also in the study on power consumption in an unbaffled bioslurry reactor (Tamburini et al., 2016). Beside high mixing efficiency, another reason for the increased popularity of this impeller type over the others is better availability of experimental data (Montante et al., 2012).
Majority of investigated stirred tanks make use of the standard design. The design is based on a vessel of a cylindrical shape with an appropriate ratio of liquid level *H* to the vessel diameter *D*. Typical ratios depend on

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an application, for instance stirred tank fermenters are mostly designed with *H*/*D* ranging from 1:1 to 3:1 (Alok et al., 2014). The stirred vessel is usually equipped with two or four baffles and a number of impellers of a diameter *d* with typical diameter ratios *D*/*d* ranging from 3 to 6. Characteristic dimensions and positions of baffles are also related to the diameter of the vessel such that the standard baffle width-to-diameter ratio *W*/*D* is 1/10 or 1/12. If gaps are left between baffles and the vessel wall, the recommended gap width-to-diameter ratio is 1/72 (Myers et. al., 2002). Baffles commonly extend from the liquid level nearly to the bottom. A type of the impeller affects the flow pattern (radial or axial). The choice of the type is upon specific needs.

1.2 Role of Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) helps to understand complexity of the (multiphase) flow in stirred tanks. It is often employed to examine various operational conditions and their effects on process parameters such as homogeneity of the mixture, residence time, impeller torque and heat and mass transfer rates. For instance, Ramírez-Goméz et al. (2013) used CFD to evaluate hydrodynamics inside a tank with either aligned or non-aligned impellers and explained a decrease of local heat transfer coefficient for the latter.
CFD also serves as a supporting tool in virtual design especially for up-scaling of chemical rectors. Unfortunately, there is no generally applicable scale-up criterion for stirred tanks (Donati et al., 1997). A choice of an appropriate criterion depends on the specific application and objectives of the scale-up. For example, Waghmare et al. (2011) developed a semi-empirical scale-up correlation using a combination of CFD and experimental techniques for the prediction of drawdown rate of solid particles in a stirred tank. In case of chemical reactors with highly exothermic reactions, it is necessary to keep temperatures in certain range by heat removal. For such applications, a Nusselt number-based criterion may be the most appropriate, as in the work of Jaimes et al. (2015), who obtained the Nusselt number values from a series of CFD simulations with a maximum variation of 15% as compared to the experimental correlation.

1.3 Objectives of the study

The present study deals with CFD simulations of a stirred tank of a nonstandard design (in terms of the shape and characteristic dimension ratios of the tank and key components). The apparatus is used in pharmaceutical industry for processing brown chicken eggshells in water flow. Current semi-batch operation (i.e. a batch of eggshells rinsed in water with continual inflow and outflow) is inconvenient and inefficient. Therefore, an upgrade is planned with scale-up of the vessel. The article reports modelling results from the first stage of the upgrade. The objective is to study multiphase flow in the batch stirred-tank and verify improvements due to extra baffling, which should improve mixing and distribution of eggshells in the entire volume. A formation of the central vortex core is studied. Up-scaling is not considered at this stage and is subject to future work.

2. Experimental unit

The current design includes an unbaffled vessel with a combined blade-helix axial impeller placed at the bottom. The absence of baffles and high rotational speed of the impeller (approx. 1440 rpm) develop strong tangential flow with a huge central vortex that reaches and reveals the impeller (based on experimental experience with the tank). Therefore mixing in the tank is not optimal and can be improved with baffling.
Main features of the stirred tank including baffling are shown in Figure 1 (left). Diameter ratios of the bottom and top cylindrical parts of the vessel to impeller are approximately 3.3 and 8.9, respectively. Designed baffles have a standard width-to-diameter ratio. However, they do not extend the bottom, which facilitates their manufacturing and installation. The pitch angle of axial blades on the impeller is 40°. The tank is filled with water to the level of 900 mm.
Experiments were performed on an industrial unit, which did not provide measurements of integral data such as pumping flow rate or impeller torque. Therefore, experimental observations only served for visual validation of the main characteristics of the water free surface such as shape and diameter of the central vortex and water level elevation on the vessel wall. Operational conditions and characteristic dimensions of the stirred tank are summarized in Table 1.

Table 1 Operational conditions and characteristic dimensions of the stirred tank.

Parameter (also see Figure 1)	Impeller speed	Ratio H/D_{top}	Ratio D_{bottom}/d	Ratio D_{top}/d	Height *H*	Width *W*	Mixing Reynolds number	Water volume
Unit	rpm	-	-	-	mm	mm	-	L
Value	1440	1.125	3.3	8.9	900	8	194000	280

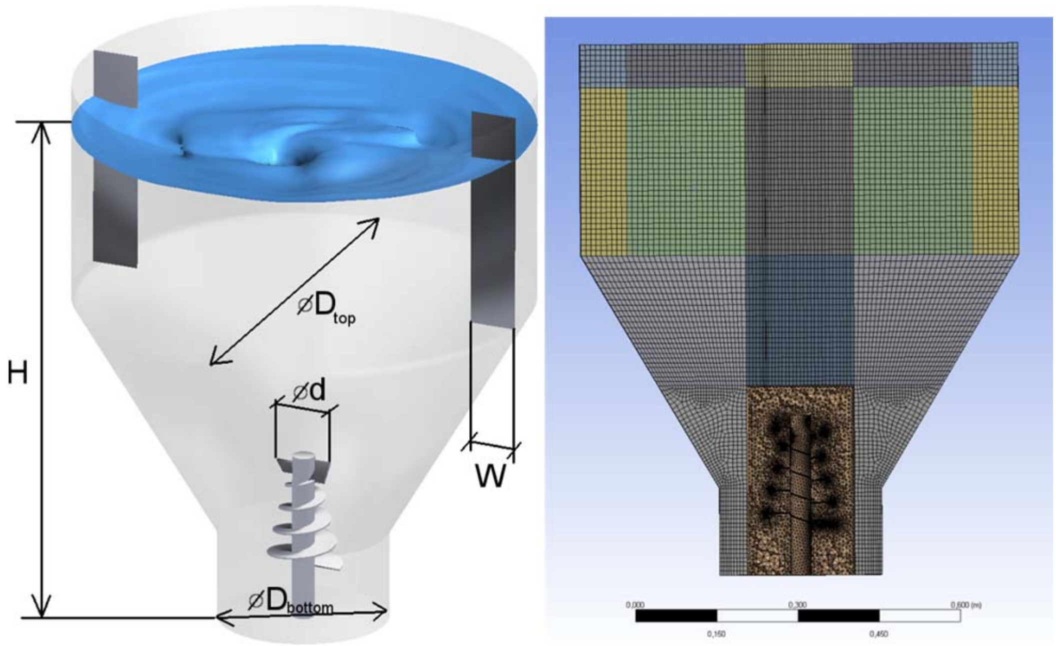

Figure 1: A sketch of the simulated baffled stirred tank (left) and axial cut of the computational grid showing local refinement near the helix of the impeller (right).

3. Computational model

A CFD model was created using commercially available software Ansys Fluent, version 17.2.

3.1 Physical models

A characteristic feature of the simulated unit is a three-phase turbulent flow, which includes water, air and solid particles. However, eggshells are very hard to characterize. First of all, it follows from published literature (Ketta et al., 2016) that an eggshell consists of several layers with different material, physical and chemical properties. Moreover, during the process, eggshells undergo structural changes due to break-up of particles and dissolution of proteins. Behaviour of such an inhomogeneous material is hard to describe for the purpose of a numerical simulation. Second, particles have highly irregular shapes. This poses an additional problem, because available modelling techniques such as Discrete Particle Model for the representation of the suspended solid phase account only for spherical particles. Deviations from spheres can be accounted for by adjusting a single parameter of sphericity, which is reflected in the drag coefficient.
Based on a measured density of 2,000 kg/m^3 of the raw eggshell and particle volume-equivalent diameters ranging from 1 mm to 15 mm, the typical Stokes numbers suggest, that most particles rather follow flow streamlines. Just a fraction corresponding to the largest particles may deviate from the flow streamlines. Hence, it was decided not to include solid particles in the present work either in experiments or in the simulations.
In order to accurately predict the deforming free surface of the stirred tank and flow in the whole liquid volume, Volume-Of-Fluid model (VOF) is enabled. Due to a turbulent nature of the flow, additional equations are necessary to describe the turbulence effects. The k-ω SST turbulence model is employed. Moving Reference Frame (MRF) approach is used to model effects of motion of impeller in the reactor. The solutions are performed as transient.

3.2 Computational grid and discretization

A computational grid is shown in Figure 1 (right). Local refinement has to be used near the helix edge with a thickness of three millimeters. The whole domain is discretized into approximately 1.3 M cells, 900,000 of which are tetrahedral and the rest are hexahedral cells.
Governing equations are discretized with the second-order upwind differencing scheme. Time derivatives are discretized using first-order implicit scheme.

4. Results and discussion

Results from three simulated cases are presented. The cases are referred to as “unbaffled” for the configuration without baffles, “baffled60” and “baffled90” for the baffled stirred tank with baffle pitched angles of 60° and 90°.

Transient solutions are computed with time steps of 0.0001 s for the unbaffled case and 0.001 s for other cases. A pseudo-steady state is reached after 20 to 30 s of operation, which is judged by monitoring temporal variation of moment of force on the impeller. Except the unbaffled case, time sampling is turned on for the next second, so the results show mean values. Results from the unbaffled case are reported by means of snapshots of time instants only. This is because as the central vortex free surface (i.e. the water-air interface) approached the region of locally refined control volumes with relatively high velocity magnitudes, the time step had to be adapted accordingly. When the interface reached the impeller, very small values of the time step were required to get converged solution. The simulation was stopped as it would take very long time to complete it.

Figure 2 shows predicted shapes of the water surface in terms of water mass fractions in vertical cuts of the tank. A huge central vortex is clearly visible in the unbaffled case. It reaches the top of the impeller in 22 s. This state has also been observed during the experiments. The time needed for the complete formation of the vortex is slightly over-predicted as compared to the experiment, where the impeller was completely revealed after 20 s of operation. Predicted water level elevation is about 30 mm as shown in Figure 3 on a detail of the vortex free surface at the vessel wall. This is in fairly good agreement with the experiment, where an elevation of 40 mm was measured by a ruler drawn at the tank wall. Note that certain amount of water volume would be removed yet by the vortex, if the impeller was completely revealed as in the experiments. Therefore, the predicted elevation of the vortex free surface at the wall would be even closer to the measured value.

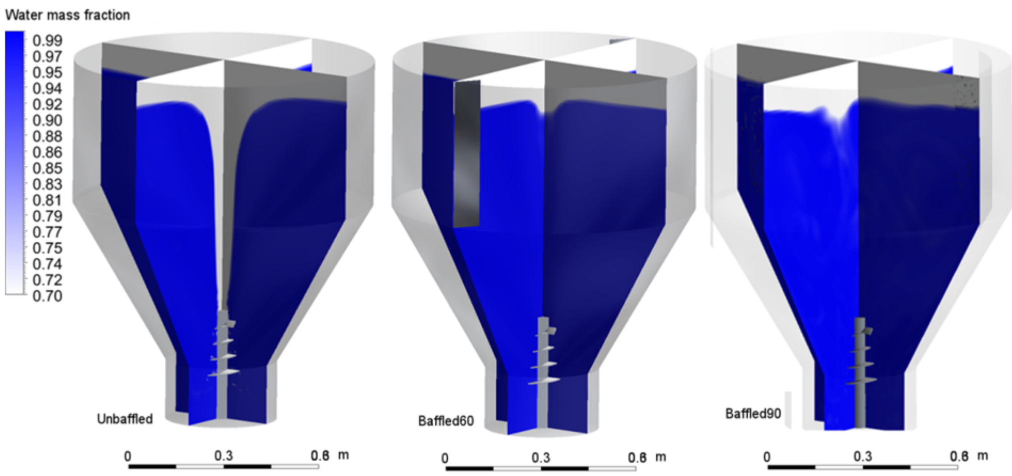

Figure 2: Shapes of the central vortex.

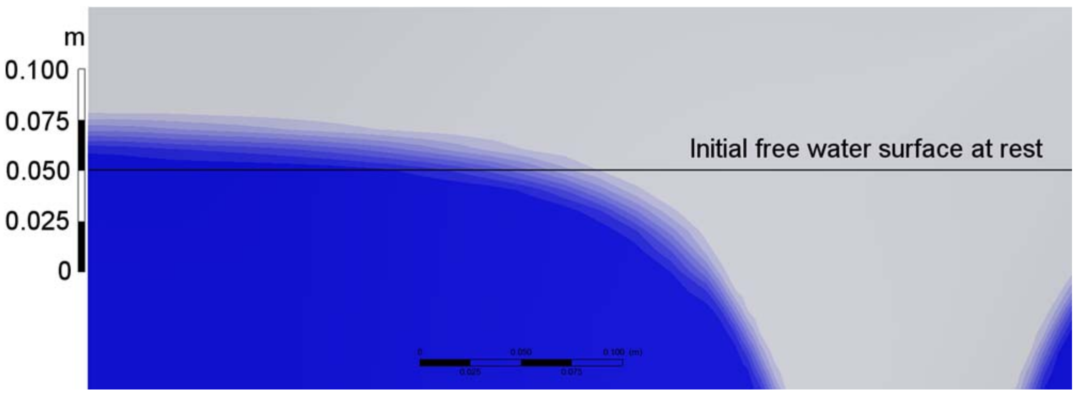

Figure 3: A detail of the elevation of the vortex free surface at the wall of the tank.

The formation of the vortex is suppressed in the other two cases due to the presence of baffling. While baffled60 still produces a small central vortex, baffled90 completely disrupts the tangential flow so that the central vortex is not formed. However, it shows an asymmetrical vortex-like structure which also appeared randomly during the experiments.
Flow patterns are more clearly seen in Figure 4 which shows vector plots in axial cuts (top) and cross-sectional cuts in a plane 300 mm below the initial water free surface. The position of cross-sectional cuts is just above the bottom of baffles, which are omitted for better clarity. Note that vectors are superimposed on the contour plots of the vortex free surface. The presence of strong tangential flow is clearly visible in the unbaffled case. Solid particles with small Stokes number would follow circular trajectories at various depths according to their mass. Unbaffled60 exhibits significant influence of both tangential and axial flows. Solids at the water surface would be drawn down to the impeller and transported back towards the surface following helical trajectories. Vectors in baffled90 case show the most intense mixing of all cases. Axial flow is the dominant flow pattern. Note that in all cases there is a small recirculation zone under the impeller helix, where large particles might accumulate. In order to reduce or avoid the accumulation, upward-pumping axial flow is recommended for the given geometry.

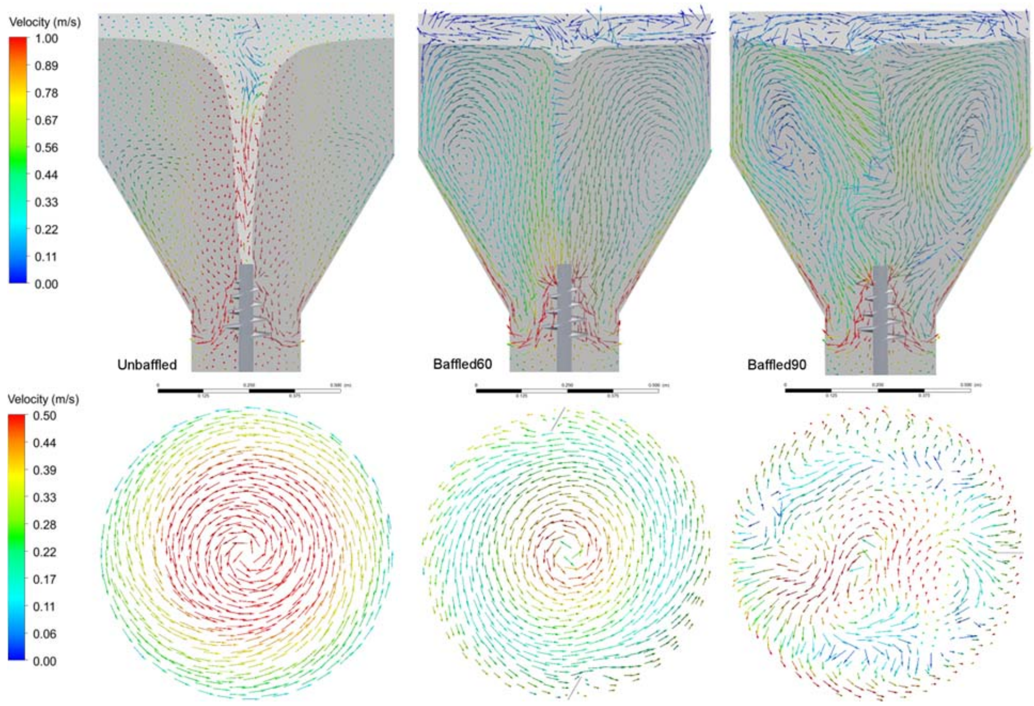

Figure 4: Velocity vector plots in axial cuts (top) and cross-sectional cuts in a plane 300 mm below the initial water level (bottom).Vectors are superimposed on the contour of the central vortex.

5. Conclusions

Results from CFD simulations of a batch-operated stirred tank are presented. Three different baffling configurations are considered including an unbaffled tank and baffling with two different pitch angels of the baffles (60° and 90°). The design of neither the stirred tank nor the inserted baffles strictly follows a common engineering practice.
Simulations confirm that an insertion of the appropriate number of baffles significantly enhances mixing in the entire volume of the tank. Although baffles are immersed from the top only to one third of the total height of the water-filled volume, they provide sufficient mixing.
Based on Stokes numbers, the flow with suspended eggshells has not been considered. However, in a typical batch mass loading, there is a fraction of large particles, for which the assumption does not hold. Vector plots also show a potentially problematic region with a recirculation zone, where larger particles might accumulate.
Future work should verify the assumption based on the Stokes number by including solid particles in the simulation. This is a challenging task in view of the facts that the eggshells are inhomogeneous material with highly irregular shapes and they undergo a number of structural changes during the process.

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