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Chemical Industry & Chemical Engineering Quarterly 16 (4) 379–386 (2010) CI&CEQ

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SCIENTIFIC PAPER

UDC 66.06:532.51

DOI 10.2298/CICEQ100211040O

CFD SIMULATION OF THE HYDRODYNAMICS AND MIXING TIME IN A STIRRED TANK

Hydrodynamics and mixing efficiency in stirred tanks influence power draw and are therefore important for the design of many industrial processes. In the present study, both experimental and simulation methods were employed to determine the flow fields in different mixing tank configurations in a single phase system. Laser Doppler velocimetry (LDV) and computational fluid dynamics (CFD) techniques were used to determine the flow fields in systems with and without a draft tube. There was reasonable agreement between the simulation and experimental results. It was shown that the use of a draft tube with a Rushton turbine and hydrofoil impeller resulted in a reduction in the homogenization energy by 19.2 and 17.7%, respectively. This indicates that a reduction in the operating cost can be achieved with the use of a draft tube in a stirred tank and there would be a greater cost reduction in a system stirred by the Rushton turbine compared to that stirred by a propeller.

Key words: Draft tube; CFD; solids concentration; stirred tank; simulation.

The performance of a stirred tank depends on mixing, which influences many chemical reaction rates as well as the product quality. For this reason, many mixing studies have been conducted in different tank configurations stirred by various types of impellers. In most of these studies, conventional impellers such as the Rushton turbine [1,2] pitched blade impellers have been employed[3,4]. Relatively few studies have been carried out using round or dished-bottomed tanks fitted with draft tubes [5,6].

A draft tube is typically employed to enhance axial mixing in stirred tanks and this promotes homogeneity. In multiphase processes, it is important to attain bed homogeneity in order to promote interphase heat and mass transfer. It has been reported [5] that draft tubes improve mixing efficiency without causing too much shear or turbulence intensity that could lead to particle attrition. In this regard, efficient mixing can be achieved by specifying optimum operating parameters such as impeller speed and phase hold up as well as design parameters. In particular, the bulk fluid flow is influenced by the liquid level above the draft tube. It was earlier reported [7] that the draft tube bottom clearance should be at least one draft tube diameter and that the highest flow per power can be obtained by this device, especially if used in a fully baffled tank. A small draft tube cross-sectional area results in a higher velocity in the core than the annulus. This leads to an increase in head loss, which is a function of the square of the fluid velocity in the draft tube [7]. Ochieng [8] reported that the bottom clearance of the draft tube should be the same as that of the impeller, especially if the impeller is a radial pumping one.

In recent studies, the revelation of many salient mixing features of multiphase systems has been possible due to the use of computational fluid dynamics (CFD) and laser Doppler velocimetry (LDV) techniques [8,9]. The information obtained from the CFD simulation of the flow field, mixing time and power is necessary for the identification of the tank dead zones, which affect mixing efficiency in a stirred tank. The mixing efficiency can be determined from homogenization energy, which is the product of the mixing time and the corresponding power dissipated [10]. A remarkable effort has been expended in simulating mixing time and power in flat-bottom tanks stirred using the Rushton turbine [11-14]. Such efforts have been constrained by the available computational power. In particular, simulation of mixing time is computationally expensive and modelling curved surfaces such as those of propeller and elliptically bottomed tank just makes the modelling work more complex. The previous authors studied the effect of draft tube

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Paper received: 11 February, 2010
Paper revised: 10 July, 2010
Paper accepted: 13 July, 2010

on flow field in a system stirred using either the Rushton turbine or a propeller. Most of the studies were done using flat bottomed tanks and, to the best on our knowledge, no comparison was made between flow field in such systems and in elliptical bottomed tanks with regards to impeller and draft tube influence. As a result, a lot of work still needs to be done in simulating such systems in order to get an insight into the mixing features therein.

More recently, Ochieng *et al.* [14] reported that at a low impeller clearance and a draft tube can improve mixing in a tank stirred by a Rushton turbine in a flat bottomed tank. It is of interest, therefore, to compare the performance of this impeller with the axial one in the same configuration and in elliptical bottom tank. The aim of the present studies is to employ both CFD and LDV techniques to study mixing time and power draw in flat and in an elliptically bottomed tank stirred by axial and radial impellers.

MODELLING

The hydrodynamics of a stirred tank are governed by the interaction between the bulk phase (liquid) flow and the tank geometry, both of which affect mixing time and energy draw. The flow field is represented by the mass and momentum balance governing equations. In the present work, the governing equations are given in a time (Reynolds) averaged form of the Navier-Stokes equations, for which the conservation of mass is:

$$\nabla \cdot (\rho U) = 0 \tag{1}$$

where ρ and U are the density and the mean velocity vector, respectively. The momentum conservation equation is given by:

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U \times U) = -\nabla \cdot p + \nabla \cdot \mu[\nabla \cdot U + (\nabla \cdot U)^T] + F_B \tag{2}$$

where p is the pressure, μ is the dynamic molecular viscosity, F_B represents body forces including Coriolis and centrifugal forces. Mixing time was calculated from the transport equation in which the transport quantity (ϕ) was the tracer mean volume fraction:

$$\frac{\partial \rho\varphi}{\partial t} + \nabla(\varphi \rho U_i) = \nabla\left[\left(\Gamma + \frac{\mu_T}{\sigma_T}\right)\nabla\varphi\right] \tag{3}$$

where Γ and μ_T are the molecular and turbulent diffusivities, respectively, σ_T is the turbulent Schmidt number. The value of σ_T is lies between 0.5 and 1, depending on the flow. In this case, after a few trials, the value of σ_T was taken as 0.7.

Power (P) exerted on the baffles was calculated as:

$$P = 2\pi MN \tag{4}$$

where M is the torque and the mean kinetic energy dissipation rate is given by:

$$\bar{\varepsilon} = \frac{P}{V_T \rho} \tag{5}$$

where V_T is the fluid volume. The homogenization energy (η) was calculated as a product of the kinetic energy dissipation rate and mixing time:

$$\eta = \bar{\varepsilon}\tau_{90} \tag{6}$$

where τ_{90} is the time required to achieve 90% homogenization. The mixing time required to achieve 90% homogenization (τ_{90}), for example, is the time it takes for the fluctuation of the response signal to be below 10% of the concentration achieved at perfect mixing.

METHODOLOGY

Hydrodynamics and mixing studies were carried out in an elliptically bottomed tank with and without a draft tube, using CFD and LDV techniques in single phase system. Detailed configuration of the mixing tank is shown in Figure 1. The fluid was water at room temperature and simulations were run using CFX--ANSYS codes [15,16]. Figure 2 shows the setup of the tank stirred by the standard Rushton turbine and the hydrofoil propeller previously employed by Ochieng [8]. The impeller diameter (D) was the same (0.33T) for both the turbine and the propeller, and the

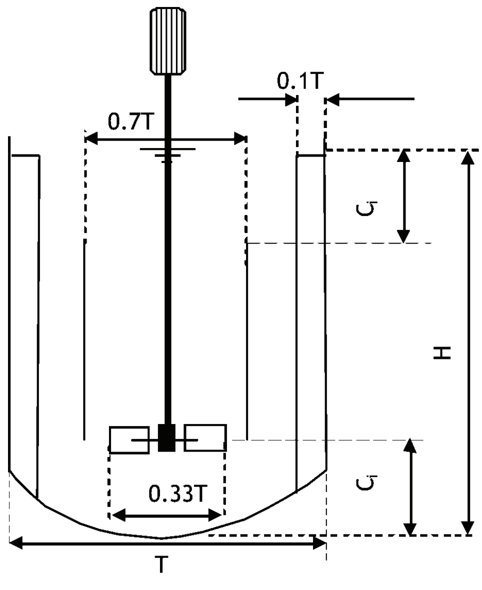


Figure 1. Reactor configuration.

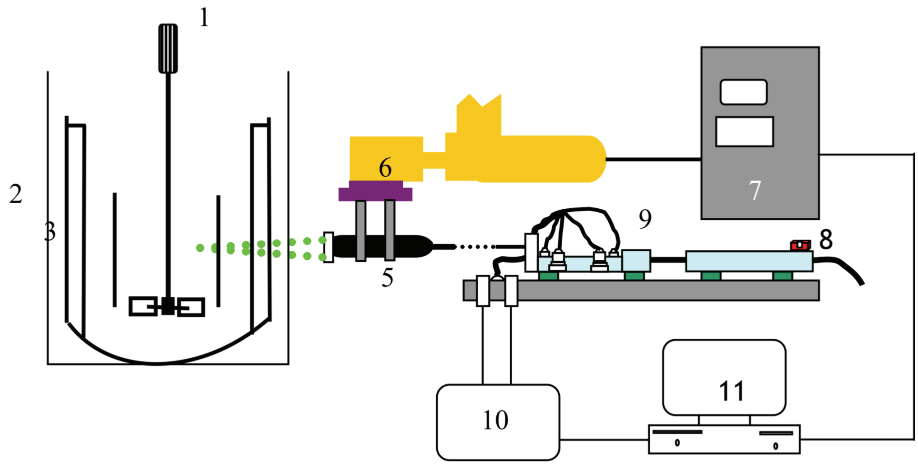


Figure 2. LDV experimental set-up.

impeller speed (*N*) was 5 rps, which corresponds to an impeller Reynolds number (*Re*) of 7.81×10^4. The tank diameter (*T*) was 0.38 m and the fluid level (*H*) was 1.3*T*. The top and bottom clearance was 0.15*T*, and the bottom clearance was the same for both impellers. The bottom clearance was taken as the distance from the centre of the hub (or the level of the disc, for the Rushton turbine) to the tank bottom.

In the configurations studied, the Rushton turbine (RT) or the hydrofoil impeller (HI) was employed with and without a draft tube. These configurations are hereafter denoted by R15T for the Rushton turbine stirred tank, in which the impeller clearance is 0.15*T*. Similarly, H15T represents the hydrofoil propeller located at 0.15*T* from the bottom. The respective systems with a draft tube (DT) are denoted by R15T-DT and H15T-DT.

EXPERIMENTAL

Figure 2 shows the LDV experimental setup for which a detailed experimental procedure has been described by Wu and Pullum [17]. The LDV probe was mounted on a robotic arm as shown in Figure 2 and the measurements of the three velocity components were taken in the middle of two baffles ($\theta = 0^{o}$). Details of the flow field determined using the LDV and mixing time determined using both decolourization and conductivity methods for similar configurations have been presented elsewhere [14,18]. The working vessel was encased in an outer transparent trough with a square cross-section, and both filled with tap water to a required depth. A conductivity meter [14] was employed to measure the mixing times that were used to validate the simulated ones. Consequently, the mixing times presented in this work are the simulated ones.

CFD Simulation

A quarter of the tank was simulated in the case of H15T while for the case of R15T, a half of the tank was simulated. For both cases, three grid sizes corresponding to half tank were used, with the total number of cells being 216000, 436000 and 700000, for the coarse, base and fine grids, respectively. The simulations were run on two P4, 2 GB memory, 3 GHz PCs using CFX5.7 codes [15,16]. For all the simulation work, the impeller shaft and the gravitational force were defined along the x-axis. The blades, disc (for the Rushton turbine) and baffles were defined as thin surfaces, and grids were refined in the wall and impeller regions. A free surface boundary condition was defined at the liquid surface, where the shear stresses were set to zero. On the walls, a no-slip condition was specified for the liquid. The standard k-ε model was employed with both the multiple frames of reference (MFR) and sliding grid (SG) approaches, both of which were developed by Luo *et al.* [19,20]. The steady state MFR approach was employed only to generate the initial result for the subsequent use in the unsteady state SG runs. The semi-implicit pressure linked equation-consistent (SIMPLEC) algorithm was used to couple the pressure and momentum equations. Equation solvers such as the block Stone and algebraic multi-grid [15] were employed with the quadratic time differencing scheme. The interconnectivity between the rotating and stationary domain was achieved by the general grid interface (GGI) algorithm [15].

Figure 3 shows the simulation domain meshed using unstructured grid, which is better than the structured grids for creating domains with high curvature. The initial simulations were run to evaluate the performance of the discretization schemes such as upwind, hybrid, higher upwind and quadratic upstream inter-

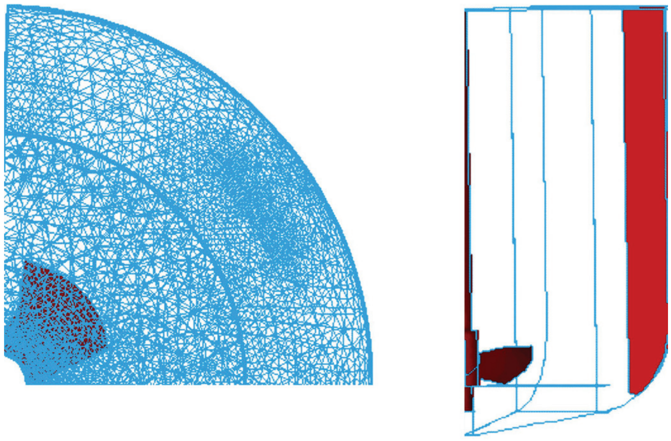


Figure 3. Modeled section showing mesh distribution: a) top view; b) side view.

polation for convective kinetics (QUICK). Full hydrodynamic equations were solved for the flow field and mixing time. Mixing time was obtained from the mean value of the mixing time obtained from five simulated probes at different part of the domain. Grid independence studies were carried out using coarse, base and fine grids. For the value of the mixing time, the difference between based and coarse grid was calculated and found to be less than 3%.

RESULTS AND DISCUSSION

Grid independence analysis showed that there was minimal difference between the base and fine grid, consequently. Subsequently, the base grids were used for the studies and a reasonable agreement between the simulation and the experimental results was obtained. The CFD simulation of the fluid flow revealed the presence of circulation loops. The orientation of the loops changed with the impeller clearance, and the centres of the loops represented dead zones, which affected both the mixing time and power draw. The draft tube was shown to improve the flow pattern and consequently, the mixing efficiency by suppressing or eliminating the loops. These observations are in agreement with the results reported by Montante *et al.* [21] and Ochieng *et al.* [14].

Discretization schemes

A very good convergence of the mass residuals up to 1.0×10^{-6} obtained with the first order discretization scheme (upwind differencing scheme) was lower than that for higher order schemes for which 10^{-5} was the minimum value obtained. However, the results obtained using the upwind scheme were a gross over-prediction of the velocity field by as much as 120%. This is an indication that the upwind results were more precise but those of higher schemes were more accurate. As a result, the data obtained using the upwind scheme was used to initialize the simulations for further runs with higher order discretization schemes. The influence of these schemes on the flow field was investigated in the upper (x = 0.8T) and lower (x = 0.21T) regions of the tank. In addition to the convergence of mass residuals, at the end of a simulation, the total mass of the traced in the domain was computed and compared with the quantity that was originally introduced into the domain, and it was found that the total mass remained the same. Further, it was ensured that the torque on the wall baffle was constant and the mass imbalance in all sub-domains was less than 1%.

It is shown in Figure 4 that there was a marginal influence of the discretization schemes on the prediction of the axial velocity profile. Figure 4a shows that the hybrid scheme gave a reasonable prediction in the lower region of the tank whilst in the upper region (Figure 4b), predictions by all three schemes were poor. However, the prediction with the hybrid scheme was, in general, better than the other two schemes. The basis of comparison was the experimental results of the flow field and mixing time as has been shown in a previous work [14].

It is shown in Figure 4 that the predictions in the impeller discharge region, in which the cell Peclet number (Pe) is higher, are better than in the top region. Due to the high cell Peclet number (which is a measure of the relative strengths of diffusion and convection) in the lower region, it is expected that the hybrid scheme effectively becomes the upwind scheme in this region. However, it is known that this first-order scheme (upwind) is prone to numerical diffusion, especially in high Reynolds flow regions like the impeller discharge region. The fact that better predic-

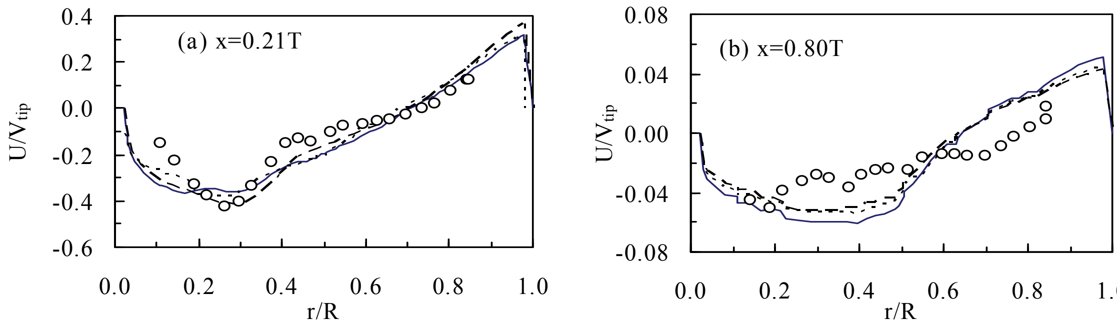


Figure 4. Effect of discretization scheme on the axial velocity profile: experiments (○), higher upwind (—), hybrid (--) and QUICK (·····).

tions were obtained with this scheme in this region suggests that the discretization schemes were not the major factors influencing the accuracy of the results. The predictions by the higher upwind scheme were better in the impeller region than in the upper tank region.

The QUICK scheme, which is third order accurate, is the most computationally demanding and the simulations in which it was used could not converge easily. Even when the residuals finally settled, the level of convergence could not go below 4.5×10^{-4}, which was the worst convergence in comparison to the other two schemes. This could be attributed to the lower diagonal dominance [22], which leads to unboundedness of the solution. A solution is unbound if it is outside the prescribed boundary conditions. For the maximum downward velocity, the higher upwind scheme gave the highest over-estimation. The maximum upward and downward velocity values give an indication of the magnitude of the circulation flow. An over-prediction of these parameters is indicative of an over-prediction of the circulation flow. The over-prediction of these parameters with the QUICK scheme in Figure 4 is in agreement with the work of Brucato *et al.* [23], in which it was reported that the QUICK scheme over-predicts the circulation rate. The maximum upward velocity was over-predicted by all schemes. In general, Figure 4 shows that the best predictions were obtained by the standard k-ε model and the hybrid scheme. Therefore, the standard k-ε model and the hybrid discretization scheme were subsequently employed.

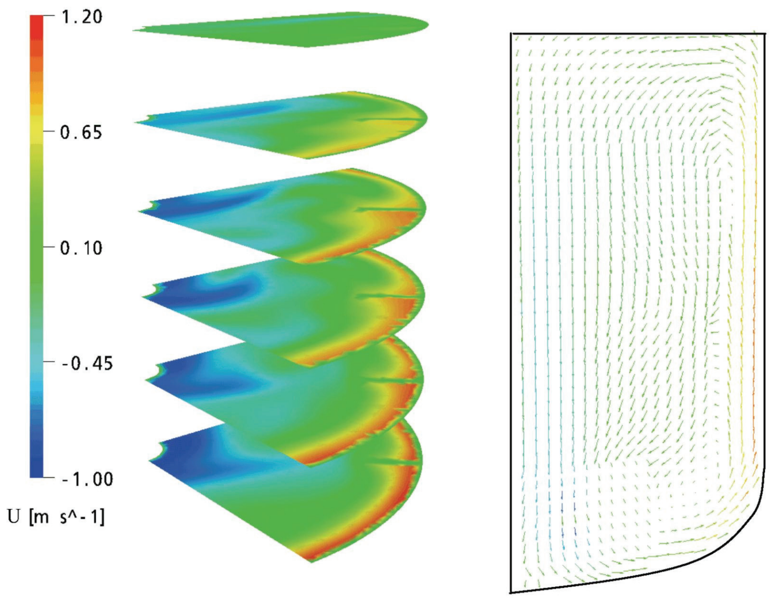
Flow field

Figure 5 shows that the secondary circulation loop that is typically found below the impellers at the standard clearance (0.33T) was suppressed. This can be attributed to the low impeller bottom clearance that was used. This observation is in agreement with previous findings [9,21]. The upward stream was confined to the region closer to the wall, and this can be attributed to the effect of the wall jet, which covered almost the entire liquid height. This is opposed to the double loop flow pattern that is characteristic on flat-bottom tanks. The upward velocity was highest in the region where r/R>0.8 and this can be attributed to the effect of the wall jet. In the region where r/R is less than 0.8, the fluid was moving downwards. Further, the axial velocity, which is dependent on the wall jet, decreased with the tank height due to the attenuation of the momentum generated by the wall jet. The uniformity of the upward and downward flow was achieved by using a draft tube for which the cross-sectional area of the core was the same as that of the annulus. This geometry results in an equal fluid velocity being attained in the annulus and draft tube where r/R = 0.7. The flow field for the configuration with a draft tube has been reported elsewhere [14].

A comparison was made between the flow generated in the flat and elliptically bottomed tanks by the Rushton turbine at a clearance of 0.15T. Simulation results in Figure 6 show that there was a higher (by 16%) axial velocity in the elliptically bottomed tank than the flat-bottomed one. This can be attributed to the elimination of the minor circulation loop at the bottom edge of the tank. These minor loops act as sinks for the momentum convective transport. In an elliptically bottomed tank, the downward impeller jet is smoothly deflected upwards rather than being partially damped as is the case in the flat-bottomed tank.

Mixing time and energy dissipation

Mixing efficiency was evaluated by calculating the homogenization energy from the dimensionless mean kinetic energy dissipation rate, $\bar{\varepsilon}$. The torque on the wall baffles was used to calculate power from Eq. (3), and this was in turn used to compute $\bar{\varepsilon}$ from Eq. (4) and the power numbers (N_p) in Table 1. The power number predictions obtained using this method were much closer to the experimental results than those obtained from the local simulation values of the turbulent kinetic energy dissipation rate. The power number for R15T was found to be 3.4, which is in reasonable agreement (12% difference) with the ex-



(a) (b)

Figure 5. Axial velocity profile in the H15T configuration: a) fringe; b) vector plots between the blades.

perimental value of 3.8 [1]. The under-prediction of the power number can be attributed to the under-prediction of the torque, which is calculated from the azimuthal momentum component. An accurate computation of this momentum depends on the tangential velocity component, which has been shown to be poorly predicted by the k-ε model [8,20]. In addition, the accuracy of the simulations based on Reynolds averaged Nervier-Stokes has been pointed out in many studies.

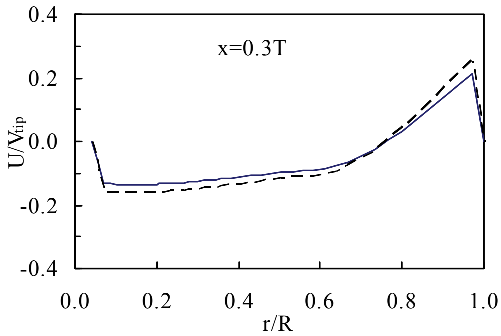


Figure 6. Comparison of the axial velocity profiles in flat and elliptically bottomed tanks, H15T: elliptical (--); flat (—).

It is apparent that $\bar{\varepsilon}$ for R15T was higher than that for H15T, and this is due to the higher power number obtained in the R15T configuration. However, most of this energy was dissipated in the lower region of the tank. The power numbers for the system with the draft tube were lower than those without. This is due to the fact that the draft tube enhances the fluid circulation, leading to a reduction in the azimuthal momentum, which is responsible for the torque on the baffles. The use of the draft tube resulted in a reduction in the homogenization energy by 19.2 and 17.7% for R15T and H15T, respectively (Table 1). In a flow generated by H15T, there are relatively less circulation loops (Figure 5) to be suppressed by a draft tube as compared to a flow generated by H15T. This could explain the slightly higher reduction of the homogenization energy in the flow generated by R15T compared to that for H15T. The Rushton turbine generally generates double loop flow pattern which is characterized by chaotic fluid flow, and this results in high energy dissipation. In contrast, the propeller (H15T) generally creates a smooth flow characterized by one major loop. As a result, the introduction of a draft tube the R15T system does not change the flow pattern as much as it does for H15T.

Table 1. Mixing time and homogenization energy simulation ($\eta = \bar{\varepsilon}\tau_{90}$) with $\bar{\varepsilon}$ from Eq. (4); N = 5 rps

Configuration	τ_{90} / s	N_p	$\bar{\varepsilon}$ / m^2 s^{-3}	η / m^2 s^{-2}	$\Delta\eta$ / %
R15T	6.47	3.40	0.09	0.59	
R15T-DT	5.94	2.75	0.08	0.48	19.17
H15T	6.04	1.11	0.06	0.35	
H15T-DT	5.65	0.92	0.05	0.29	17.74

CONCLUSION

Hydrodynamics and mixing in a stirred tank was investigated using computational fluid dynamics (CFD) simulation and laser Doppler velocimetry techniques. The influence of a draft tube on mixing time and power draw was studied in flat and in an elliptically bottomed tank stirred by axial and radial impellers. In the CFD application, the effect of discretization schemes (first and higher order schemes) on the simulation results was investigated. The results obtained using the hybrid discretization scheme, compared to experimental data, were as good as or better than those of the third-order accurate upwind scheme (QUICK). This shows that a higher-order scheme does not necessarily give better predictions for the systems investigated. The use of a draft tube resulted in higher (19.2%) homogenization energy reduction in the Rushton turbine stirred tank than that (17.7%), in the hydrofoil impeller stirred tank. This is an indication that a reduction in the operating cost can be achieved with the use of a draft tube.

Acknowledgement

Contributions by Prof. Alison E. Lewis and Dr Paul Musonge are gratefully acknowledged.

Symbols

CFD	Computational fluid dynamics
D	Impeller diameter, m
F_c	Centrifugal force, N
F_{ce}	Coriolis force, N
H	Fluid depth, m
k	Dimensionless turbulent kinetic energy
LDV	Laser Doppler velocimetry
M	Torque, N m
MFR	Multiple frame of reference
N	Impeller speed, s^{-1}
P	Power, W
p	Pressure, kPa
Pe	$\rho ul/(\Gamma\Delta x)$
R	Ratio of the diameter of the draft tube to that of the column
r	Tank radius, m
SG	Sliding grid
t	time, s
T	Tank diameter, m
U	axial velocity, m/s
V_{tip}	Impeller blade tip velocity, m/s
x_i	Cartesian coordinates
Δx	Dimensionless cell width

Greek symbols

$\bar{\varepsilon}$	Mean specific kinetic energy dissipation rate, $m^2 s^{-3}$
η	Homogenization energy, $m^2 s^{-2}$
μ	Molecular viscosity, kg $m^{-1} s^{-1}$
ν	Viscosity, $m^2 s^{-1}$
ρ	Density, kg m^{-3}
Γ	Diffusion coefficient, kg $m^{-1} s^{-1}$

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NAUČNI RAD

SIMULACIJA HIDRODINAMIKE I VREMENA MEŠANJA U SUDU SA MEŠANJEM POMOĆU RAČUNARSKE TEHNIKE STRUJANJA FLUIDA

Hidrodinamika i efikasnost mešanja u sudovima sa mešanjem utiču na snagu mešanja, pa su zbog toga značajni za projektovanje mnogih industrijskih procesa. Da bi se odredila strujna polja u sudovima različite konfiguracije, u ovom radu su korišćene i eksperimentalne i simulacione metode. Tehnika merenja brzine laserskim Doplerom (LDV) i računarska tehnike simulaije strujanja fluida (CFD) su primenjene radi određivanja strujnih polja u sistemima sa i bez centralne cevi. Utvrđeno je prihvatljivo slaganje između simulacija i eksperimentalnih rezultata. Upotrebom centralne cevi u kombinaciji sa Raštonovom turbinskom mešalicom ili propelerskom mešalicom tipa Hydrofoil smanjuje se potrebna energije za homogenizovanje za 19,2 i 17,7%, respektivno. Ovo ukazuje da se smanjenje u operativnim troškovima može postići upotrebom centralne cevi u sudu sa mešanjem, kao i da će se troškovi više smanjiti u sistemu sa Raštonovom turbinskom mešalicom nego u sistemu sa propelerskom mešalicom.

Ključne reči: centralna cev; CFD; koncentracija čvrste faze; sud sa mešanjem; simuacija.