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NUMERICAL INVESTIGATION OF INTERNAL FLOW IN STIRRED TANKS

Bruno Manoel Pasquim
Viviana Cocco Mariani
Pontifícia Universidade Católica do Paraná - Rua Imaculada Conceição, 1155, CEP: 80215-901, Curitiba - PR - Brasil
bruno.pasquim@pucpr.br
viviana.mariani@pucpr.br

Abstract. *Mixing of single and multi-phase fluids is frequently performed in stirred tanks which is one of the most basic unit operations in the chemical and bio-technology industries in applications such as liquid–liquid contactors, particle suspensions, polymer reactors, etc. An understanding of the flow behavior within the stirred vessel is essential for equipment design, process scale-up, energy conservation, and product quality control. The present study investigate the behavior of the three dimensional flow of water, considering a Stirred Tank with a Rushton Turbine. To perform such analysis the ANSYS CFX version 13 software will be used for the numerical solution of the governing equations. Inadequacy of industrial mixing equipment and not appropriate operating conditions can adversely affect process performances therefore this area needs more extensive, systematic and profound studies.*

Keywords: Stirred tanks, Computational fluid dynamics, heat transfer, turbulent flow.

1. INTRODUCTION

Mixing of single- and multi-phase fluids is frequently performed in stirred tanks which is one of the most basic unit operations in the chemical and bio-technology industries in applications such as: liquid–liquid contactors, particle and droplet suspensions, polymer reactors, etc. An understanding of the flow behavior within the stirred vessel is essential for equipment design, process scale-up, energy conservation, and product quality control and can only be achieved by simulation and analysis of the multi-scale complex fluid dynamics involved in the mixing process (ALEXOPOULOS et al., 2002).

The mixing process is used in different sectors of industry for various purposes: bend miscible liquids, immiscible liquids mix (production of emulsions), gas dispersion on liquid (aeration), reducing agglomerates of particles, accelerate chemical reactions and improve the fluid heat exchange with the tank wall.

Some variables of the mixing process can be change according with necessity and kind of process to improve the equipment performance, such as impeller velocity, vessel geometry and mainly impeller geometry. Thanks to process evolution and constant need for performance and quality improvements, many agitators were studied as in Delaplace et al. (2001), Letellier et al. (2002), Alliet-Gaubert et al. (2006) and Aubin and Xuereb (2006).

Apart from the mixture, the heat transfer inside the vessel is very important, being subject to decades of research, according Mohan et al. (1992), the process usually depend of temperature, the knowledge about heat transfer is critical equipment design. Ludwig (1999) said that the technical and economic performance of stirred vessels designs must to be checked to ensure a good cost-effective equipment that will be the "heart" of some industries.

The heat transfer in a stirred tank is usually performed through the vessel wall, Engeskaug et al. (2005) said that heat transfer coefficient depends on a number of factors such as: vessel and impeller geometry, impeller position, turbulence intensity and fisical properties of the system.

The study of the flow in stirred tanks is performed at decades, Askew and Beckmann (1965) conducted a experimental study and local coefficients of heat exchange and mass were determined, afterwards Suryanarayanan et al. (1976) and Balakrishna and Murthy (1980) study stirred tanks, furthermore experimental methods can neither cover all relevant parameters involved in the mixing process, once they become more expensive with complexity increased of the problem, instability of the turbulent flow, complex geometry, etc. (ALEXOPOULOS et al., 2002).

Detailed analysis of the large amount of data generated by CFD (Computational Fluid Dynamics) simulations can reveal flow behavior, circulation patterns, vortex structures and, at a smaller scale, turbulence intensity, dissipation rates, Reynolds stresses, etc (ALEXOPOULOS et al., 2002).

Because of the low cost of numerical methods and the evolution of computer processing equipment, the CFD becomes more common in the last 2 decades, emphasized by the commercial software expansion dedicated to this purpose.

Studies of stirred tanks were performed using computer simulation by Dong et al. (1994), Ciofalo et al. (1996), that worked in cylindrical stirred tanks with radial impellers, Sahu et al. (1998) include equally spaced baffles in the vessel wall increasing the turbulence flow, Montante et. al (2001) and more recently Alcamo et al. (2005) studied the flow behavior in the stirred tank with Rushton Turbine as impeller, as the present work. New works include the flow study

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with a tracer injection and shows how the agitation promotes fluid incorporation and tank homogenization, such as Javed et al. (2006) and Torré et al. (2008), or the mixture between fluid and solid particles in Hosseini et al. (2010). All work aims to understand the fluid's behavior in industrial reactors and thereby optimize their designs.

2. BRIEF BIBLIOGRAPHICAL REVIEW

Liquids are most often agitated in some kind of tank or vessel, usually cylindrical in form and with a vertical axis. The top of the vessel may be open to the air; more usually it is closed. The proportions of the tank vary widely, depending on the nature of the agitation problem (McCABE et al., 1993).

Mixer performance is often related in terms of the fluid velocity during agitation, total pumping capacity (flow of the fluid in the system) generated by one impeller, and the total flow in the tank (or sometimes as blending time or a solids-suspension criterion) (LUDWIG, 1999).

The fluid velocity inside the vessel have three components, the radial velocity (V_r) that act in the perpendicular direction of the agitator shaft, longitudinal direction (V_z) that act in parallel direction of the agitator shaft and the tangential or rotational velocity (V_θ) that represents a circular motion around the agitator shaft.

There are many impeller geometries, and these geometries vary according to the type of process. According McCabe et al. (1993) the three main types of impellers are propellers, paddles, and turbines and represent 95 percent of all liquid-agitation problems, a few of these impellers are presented in Fig. 1.

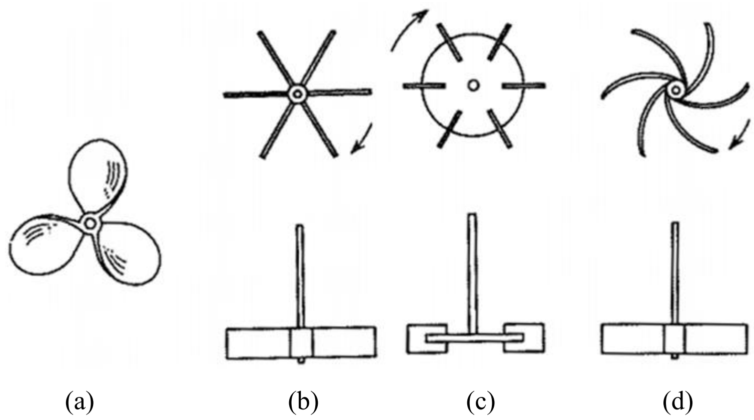

Figure 1 – Top and front view of the most common types of impellers, three-blade marine propeller (a), open straight-blade turbine (b), bladed disk turbine or Rushton Turbine (c), Vertical curved-blade turbine (d).
Fonte: Adpted from McCABE, 1993.

The flow field generated by an impeller in a stirred tank with a single phase fluid are useful to verify the presence of dead (stagnant) zones inside the tank. Too the mixing efficiency, as wel as the product quality is influenced by flow patterns in the vessel (COULSON and RICHARDSON, 1999).

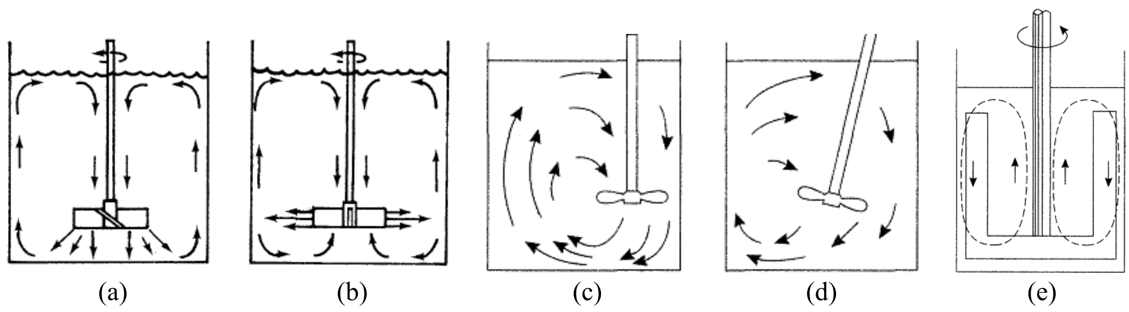

Figure 2 – Liquid flow patterns with a piched-blade turbine (a) open straight-blade turbine (b) decentralized impeller (c) prone and decentralized impeller (d) and anchor impeller (e).
Source: Adapted from LUDWIG, 1999; COULSON and RICHARDSON, 1999.

Examples of flow patterns are show in Fig. 2, where the variation created in the flow with the different kinds of impellers can be observed. The impellers in Fig. 2a and Fig. 2b created vortex in the center of the tank, this flow can make the air above the tank is mixed with the product which is often not desired, one alternative to reduce this king of vortex is change the position of the impeller, as show in Fig. 2c and Fig. 2d.

ISSN 2176-5480

The mixing equipment can be design simply as a means of achieving a desired degree of homogeneity but it may also be used to promote heat and mass transfer, often where a system is undergoing a chemical reaction (COULSON e RICHARDSON, 1999).

The intensity of heat transfer during mixing of fluids depends on the type of the agitator, the design of the vessel and conditions of the process (KARCZ e STRĘK, 1995).

3. PROBLEM FORMULATION

3.1 Geometry

With the aim of validate the numeric methodology, as well determinate the best mesh to numeric simulations, was used the symmetric geometry show in a cross-section in Fig. 3 and studied by Alcamo et Al. (2005), the dimensions are presented in Tab. 1.

Table 1. Dimensions of stirred vessel.

Parâmetros	Dimensões (mm)
Tank diameter (*T*)	190
Tank height (*H*)	T
Impeller diameter (*D*)	T/2
Impeller blade width (*a*)	D/4
Impeller blade weight (*b*)	D/5
Impeller base diameter (*d*)	3/4 D
Impeller clearance (*C*)	T/3

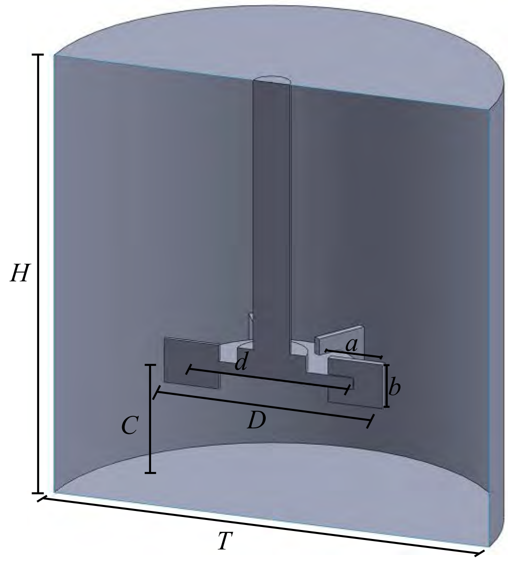

Figure 3. Stired vessel cross-section view.

The stirred tank presents diameter *T* and height *H* was used a impeller type Rushton Turbine with diameter *D* and six rectangular blades equally spaced and same size ($a \times b$), located in the center of the tank to a height *C* of the bottom. The surface of the walls and blades were considered non-slip.

3.2 Governing Equations

A 3D steady flow generated by an axial flow impeller, Rushton Turbine, in a cylindrical vessel was considered. The standard k-ε turbulent model was chosen for numerical simulation. A cylindrical coordinate system was used, with origin located at the vessel center and height H=0, the angular position θ=0 coincided with one of the impeller blades. The equations to be solved are the mass and momentum equations for a constant-density fluid in turbulent motion, which, in cylindrical co-ordinates *r*; and *θ z*, have the form:

$$\frac{\partial}{\partial z}(\rho V_z) + \frac{1}{r}\frac{\partial}{\partial r}(\rho r V_r) + \frac{1}{r}\frac{\partial}{\partial \theta}(\rho V_\theta) = 0, \tag{1}$$

the axial momentum equation becomes,

$$\frac{1}{r}\left[\frac{\partial}{\partial z}(\rho r V_z V_z) + \frac{\partial}{\partial r}(\rho r V_r V_z) + \frac{\partial}{\partial \theta}(\rho V_\theta V_z)\right] = -\frac{\partial p}{\partial z} + \frac{1}{r}\left\{\frac{\partial}{\partial z}[r(\sigma_{zz} - \rho\langle v_z v_z\rangle)] + \frac{\partial}{\partial r}[r(\sigma_{zr} - \rho\langle v_z v_r\rangle)] + \frac{1}{r}\frac{\partial}{\partial \theta}[r(\sigma_{z\theta} - \rho\langle v_z v_\theta\rangle)]\right\}, \quad (2)$$

and the radial momentum equation becomes,

$$\frac{1}{r}\left[\frac{\partial}{\partial z}(\rho r V_z V_r) + \frac{\partial}{\partial r}(\rho r V_r V_r) + \frac{\partial}{\partial \theta}(\rho V_\theta V_r)\right] - \frac{\rho(V_\theta + \Omega.r)^2}{r} = -\frac{\partial p}{\partial r} + \frac{1}{r}\left\{\frac{\partial}{\partial z}[r(\sigma_{zr} - \rho\langle v_z v_r\rangle)] + \frac{\partial}{\partial r}[r(\sigma_{rr} - \rho\langle v_r v_r\rangle)] + \frac{1}{r}\frac{\partial}{\partial \theta}[r(\sigma_{r\theta} - \rho\langle v_r v_\theta\rangle)]\right\} - \frac{(\sigma_{\theta\theta} - \rho\langle v_\theta v_\theta\rangle)}{r}, \quad (3)$$

and finally the tangentially momentum equation is,

$$\frac{\partial}{\partial z}[\rho V_z(rV_\theta)] + \frac{1}{r}\frac{\partial}{\partial r}[\rho r V_r(rV_\theta + \Omega r^2)] - (\Omega r^2)\frac{1}{r}\frac{\partial}{\partial r}(\rho r V_r) + \frac{1}{r}\frac{\partial}{\partial \theta}[\rho V_\theta(rV_\theta)] = -\frac{\partial p}{\partial \theta} + \frac{\partial}{\partial z}[r(\sigma_{z\theta} - \rho\langle v_z v_\theta\rangle)] + \frac{1}{r}\frac{\partial}{\partial r}[r^2(\sigma_{r\theta} - \rho\langle v_r v_\theta\rangle)] + \frac{1}{r}\frac{\partial}{\partial \theta}[r(\sigma_{r\theta} - \rho\langle v_\theta v_\theta\rangle)], \quad (4)$$

where V_z, V_r and V_θ are the ensemble averaged velocities. The stresses σ_{ij} are the viscous shear stresses, while $\langle v_z v_z \rangle$, $\langle v_r v_r \rangle$, $\langle v_\theta v_\theta \rangle$, $\langle v_z v_r \rangle$, $\langle v_z v_\theta \rangle$ and $\langle v_r v_\theta \rangle$ are the ensemble averaged Reynolds stresses. The turbulent transport is approximated by the k-ε turbulence model. Details about the equations can be found in Dong et al. (1994).

3.3 Boundary Conditions

Water was used for the simulation of turbulent flow in Steady State, whose properties are described in Table 2~~Table 2~~.

Table 2. Fluid properties.

Water	Temperature (*t*)	25 ºC
	Specific mass (*ρ*)	997 kg/m³
	Pressure (*P*)	1 atm
	Viscosity (*μ*)	0.001003 kg/m.s
	Specific Heat (*cp*)	4,182 J/kg.K
	Thermal Conductivity (*k*)	0.6 W/m.K

The impeller was considered an immersed solid in the fluid with rotation velocity *Vtip* = 200 rpm or 1 m/s, the vessel was considered with no slip and smooth walls.

3.4 Numerical Methodology

The set of coupled partial differential equations presented in the previous section was solved using the element-based finite volume method (PATANKAR, 1980), with the use of the commercial CFD package ANSYS CFX 13.0.

The ANSYS CFX is used to simulate different types of flow, with ANSYS it's possible build geometry, mesh, adjust simulation parameters, solve the set of equations and analyze the results. This commercial software works, sometimes, as a "black box", disabling changes and even understanding of its program structure. However shows a good interface software-user, and the user has the possibility to include computational sub-routines written in FORTRAN language. Furthermore, presents the flexibility of the inclusion of equations to compute some variables (SUSIN, 2007).

Recent advances in computing power, together with powerful graphics and interactive 3D manipulation of models, have made the process of creating a CFD model and analyzing results much less labor intensive, reducing time and, hence, cost. As a result of these factors, Computational Fluid Dynamics is now an established industrial design tool, helping to reduce design time scales and improve processes throughout the engineering world. CFD provides a cost-effective and accurate alternative to scale model testing, with variations on the simulation being performed quickly, offering obvious advantages (User's Manual Version 13.0, 2010).

CFD is used by engineers and scientists in a wide range of fields. According the ANSYS CFX User's Manual Version 13.0 the typical applications include:

- **Process industry:** Mixing vessels, chemical reactors
- **Building services:** Ventilation of buildings, such as atriums

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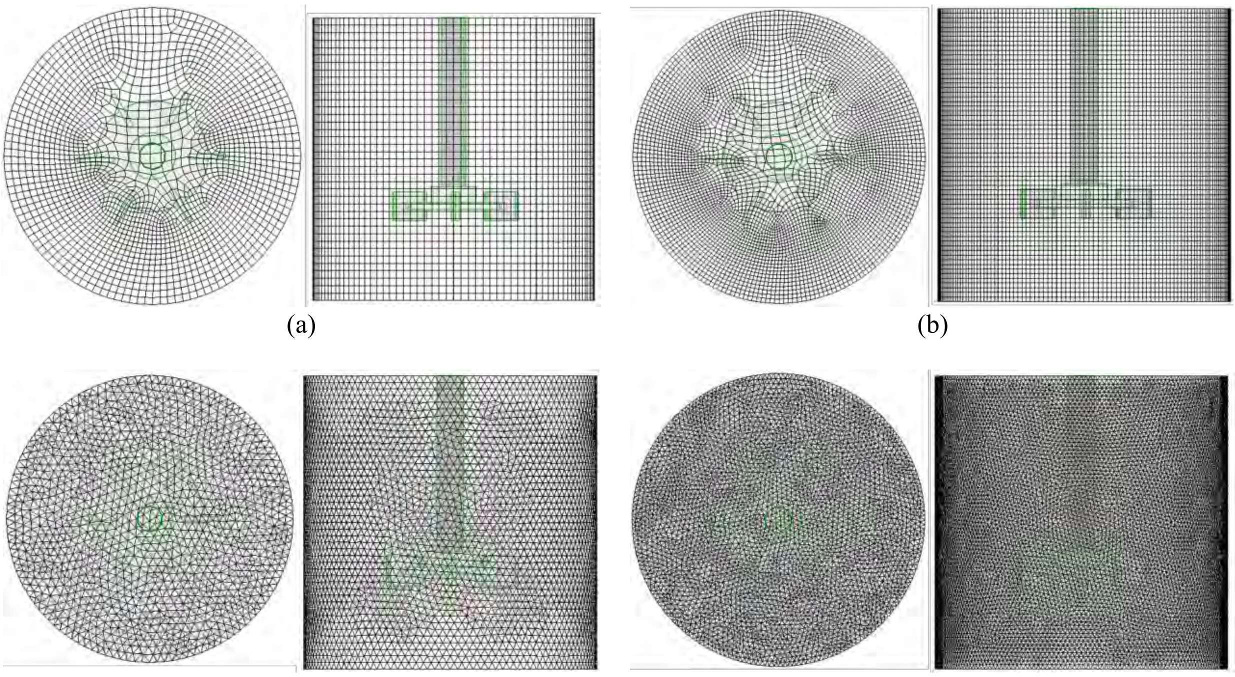
- **Health and safety:** Investigating the effects of fire and smoke
- **Motor industry:** Combustion modeling, car aerodynamics
- **Electronics:** Heat transfer within and around circuit boards
- **Environmental:** Dispersion of pollutants in air or water
- **Power and energy:** Optimization of combustion processes
- **Medical:** Blood flow through grafted blood vessels

4. RESULTS AND DISCUSSIONS

The simulations were performed for the complete geometry (no symmetry),where were used four computational meshes, as shown in Fig. 4.



(a) (b) (c) (d)

Figure 4. Mesh 1 (a), Mesh 2 (b), Mesh 3 (c) and Mesh 4 (d).

Hexahedral elements have a priority in meshes 1 and 2, while the meshes 3 and 4 show mainly tetrahedral elements, the number of nodes and elements of each mesh are presented in Tab. 3.

Table 3. Meshes properties.

Mesh	Nodes	Elements
1	79,423	77,991
2	288,791	291,584
3	154,266	383,207
4	459,123	1,184,356

The results of the simulations in the four meshes was evaluated using lines of dimensionless tangential velocity ($V_\theta/Vtip$) through the dimensionless radial direction (r/R), where r is the position and R is the tank radius ($T/2$). The profiles are shown for four different elevations of the stirred tank as shown in Fig. 5, the results are presented in Fig. 6 and compared with Vella et al. (2003).

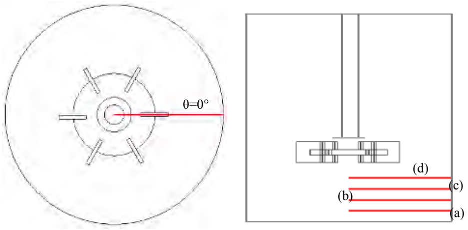


Figure 5. Positions of radial lines of tangential velocity, $\theta = 0°$ (a) $z/T = 0.053$; (b) $z/T = 0.105$; (c) $z/T = 0.158$; (d) $z/T = 0.211$

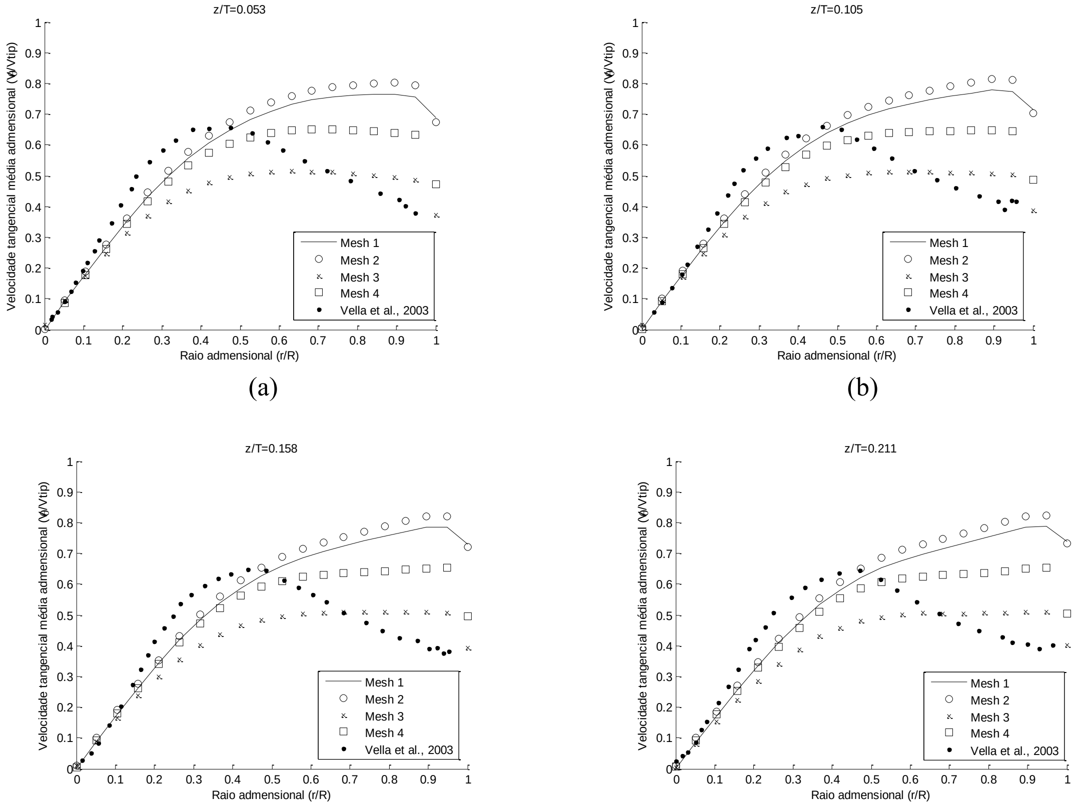


Figure 6. Radial profiles of tangential velocity at different elevations.

The meshes 1 and 2, less refined, show higher values of tangential velocity of fluid in the wall, with the meshes refine, meshes 3 and 4, the tendency is obtain lower velocities on the wall. Considerable differences are found between the results obtained and results of the reference paper, the peak of velocity observed Vella et al. (2003) near to the tank center (r/R = 0.45) and the declining of the velocity until the wall wasn't observed in the simulations, but with the meshes refine the results becomes closer.

Reports of instantaneous velocity vector are shown in Fig. 7. These results were plotted in the same instant, with developed flow, and at three azimuthal locations relative to a blade: plane containing the blade (a); 15° behind the blade (b); and 40° behind the blade. The higher intensity of the radial flow was observed at the plane containing the blade, at all the planes the tendency of the fluid flow in the center of the tank, near the impeller shaft, toward the bottom, and flow to top of the tank near the walls, as in Vella et al. (2003). Many recirculations were observed through of the tank, and the more pronounced are positioned immediately above and below the agitator. The center of the tank has a lower intensity of velocity vectors, which may represent a zone of stagnant or low flow.

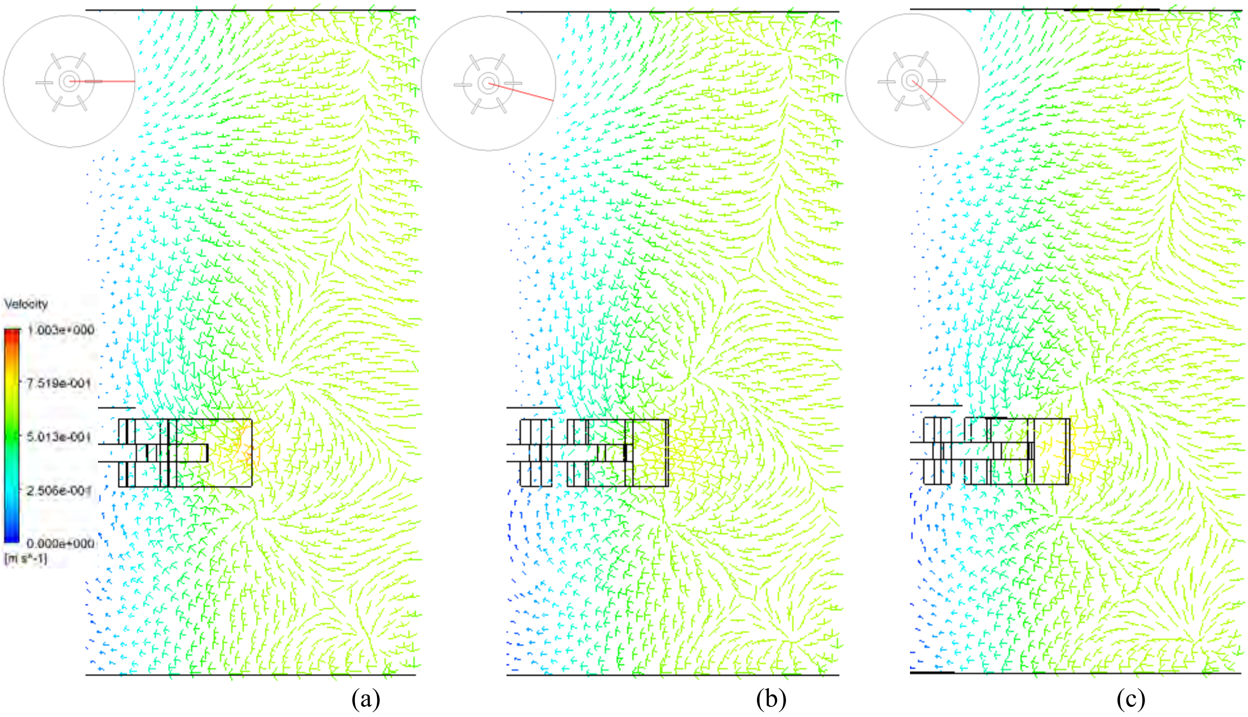


Figure 7. Instantaneous velocity vector plots at three azimuthal locations relative to a blade: (a) plane containing the blade (b) 15° behind the blade (c) 40° behind the blade;

5. CONCLUSIONS

The turbulent flow generated in a tank with 190 mm of diameter with a Rushton Turbine impeller was simulated applying the k-ε model of turbulence and helped by the commercial software ANSYS CFX 13.0. There is the need ti improve the results to flow of fluid near the walls and the edges of impeller, zone with higher intensity of flow.

No satisfactory results were obtained compared to the experimental results presented by Vella et al. (2003), as a next step improve the mesh refinement near the walls of the tank, so as to perform simulations with other models of turbulence available in the software.

The next steps of the work are study the flow non isothermal simulating a jacket vessel with heating in the walls, verifying the temperature gradient and the warming impact on the fluid flow.

6. ACKNOWLEDGMENTS

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