CFD Investigation of Impact of Vessel configuration and Different Impeller Types in Stirred Tank

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Abstract. Computational Fluid Dynamics (CFD) study is carried out to simulate the flow characteristics of different impeller types in stirred tanks of baffled and un-baffled system. The hydrodynamic behavior induced by a Rushton turbine (RT6) and Curve Blade impeller (CD-6) is numerically analysed by solving the Navier-Stokes equations coupling with $k$-$\varepsilon$ turbulence model with Multi-reference frame (MRF) impeller model. The predicted results were validated with available experimental published data and show a satisfactory agreement. The power characteristics for the two agitator systems (baffled and un-baffled) were obtained for the turbulent system of the fluid flow. In these conditions, it is found that the power number depended strongly on the length of the baffle when baffled is provided. Therefore, the presence of the baffles in the tank greatly improved the mixing performance of the system but consumes higher power than the un-baffled system. Similarly, mixing improves when Rushton impeller is employed but consumes higher power than the Curve Blade impeller. Hence, it was observed that overall efficiency of the system is better when baffled system of Curve Blade impeller is opted in any mixing operation.

1. Introduction

The capability of Computational fluid dynamics (CFD) as a powerful tool for the design of and scale-up of mechanically stirred reactors has been reported by many researchers e.g. [1-4]. In recent years, CFD techniques are being increasingly used as a substitute for experiments to obtain the detailed flow field for a given set of fluid, impeller and tank geometries [5]. Computational fluid dynamics (CFD) is an accepted and well-used means of assessing and optimizing process designs without necessarily incurring the expense of prototype development [6]. Advantage of CFD based prediction methods is that it does not have scaling up or scaling down problems as it solves the fundamental equations governing fluid flow [4]. CFD is a powerful tool for investigating flows at low cost when it is required by a high-quality experimental facility [7]. It is suggested by [2] that for accurately predicting the turbulence in the system, ‘computationally intensive’ conditions must be adopted but for studying the mean fluid flow ‘computationally light’ conditions may be applied in the simulation.

Most industrial stirred vessels are often used baffles in the system so that breaking of the undesired tangential velocity components can occur avoiding the pronounced central vortex formation at high angular speeds. It is expressed by [8] that the presence of baffles increases the circulation of velocities (axial and radial) which enhances better mixing performance in the system than the un baffled system. Even though baffled systems are commonly used in several applications, for specific purposes unbaffled systems are also desirable. It is argued that if baffled is removed, the whole fluid flow characteristics will change and hence impacting to the performance of the system [9]. Therefore, Unbaffled systems are used for specific purposes if the presence of baffled results into drawbacks [10]. It is found out by [8] one drawback of baffled system that it actually worsens the mixing performance in the aeration process because of formation of dead zones at certain regions in the system. For example, in the food and pharmaceutical industries, it is necessary to keep the system clean as much as possible therefore formation of dead zone is undesirable and in biological applications [11] shear and impact are to be reduced up to certain limit. Likewise, in crystallization
processes [12] and; in precipitation processes baffles may suffer from incrustation problems [13]. Scientific literature shows an increasing interest towards unbaffled stirred vessels: both experimental investigations [14-20] and computational studies [21-23, 9,10, 19]. It was found by [19] that the minimum power requirements for complete suspension in top-covered unbaffled vessels are lower than those in corresponding baffled tanks.

Standard impeller (Rushton) is commonly used but several researchers have shown its inferiority in performance [24-33] as compared with other types of impeller. Concave type blade was introduced by [35] modifying from the flat type blade keeping in mind to improve the performance of the system. Consequently, less than about 50% of the installed power of the motor is put to effective use during normal operations in such curve/concave blade type.

The objective of this work is to employ CFD technique to study the mixing operation of different impeller designs. It was also anticipated that this work would give an essential basis for accurate scale-up of mixing systems in industrial, field, and various type of agricultural mixing operations. In this study, different types of impellers: Curve blade and Rushton turbine impellers were designed and studied to deduce how their different design attributes will impact the flow characteristics. Velocity profiles generated in CFD were interpreted as the impeller flow characteristics. The standard k-epsilon ($\varepsilon$) model was used for modelling the turbulent flow process and the multiple reference frames (MRF) technique was employed to model the impeller motion in a baffled tank.

2. Stirred tank configuration
The first configuration we considered is that of a cylindrical tank equipped with a Rushton turbine (Fig.1a). The second is a fully baffled tank (Fig.1b). The height of the cylindrical tank is equal to its diameter (T=H), and the baffle thickness is defined by w=H/10. Impeller is placed in the axial position corresponding to z=H/3, and has diameter d=T/3.

![Fig.1: Stirred Tank Configuration for (a) Unbaffled Tank and (b) Baffled Tank](image)

The types of impeller i.e., Rushton and Curve blade used in this study are presented in Fig.2. The length of blade ($l = d/4$) and width of blade ($b = d/5$) is provided. The number of blade used is six and curvature of the Curve blade is provided as 140°.
3. Numerical Simulation

In CFD simulation two main equations are involved as continuity and momentum equation. These equations describe the motion of fluid substances and are solved by iteration process in CFD simulation. In the main momentum equation, one more term called Reynolds stresses (velocity component) by averaging the mean and fluctuating velocity is added, and the new equation is known as RANS (Reynolds Averaged Navier-Stokes) equations. To solve this Reynolds stresses, several turbulence models (k-ε; k-ω; Large eddy simulation, LES; Reynolds stress model, RSM; etc.) are available based on certain assumptions. Therefore, the basic theoretical fundamentals and equations (ANSYS, 2017) involved in the numerical simulation using CFD techniques will be presented in this section. Basic numerical equations solved in the CFD simulation are categorized as governing equations and turbulence model equation. The other numerical models & criteria to be adopted such as mesh generation (impeller model, discretization scheme), convergence criteria, boundary condition, etc. is also presented in this section.

3.1 Governing Equations

3.1.1 The Continuity Equation. Continuity equation in conservation form obtained by applying the principle of conservation of mass on a control volume fixed in space and described in differential form is:

$$\frac{\partial \rho}{\partial t} + \nabla . \rho \vec{u} = 0$$  \hspace{1cm} (1)

Where, $\vec{u}$ is the flow velocity at a point on the control surface, and $\rho$ is the density of fluid. For incompressible flows, Eq. (1) is simplified to

$$\nabla . \vec{u} = 0$$  \hspace{1cm} (2)

3.1.2 The Momentum Equation. The conservation form of momentum equation by the application of Newton’s second law of motion to a fixed fluid element is described by three scalar equations corresponding to x, y and z directions and for viscous flows they are termed as Navier – Stokes equation. The conservation form is described as:

$$\left[ \frac{\partial \vec{u}}{\partial t} + (\vec{u} \nabla) \vec{u} \right] = -\nabla p + \nabla \cdot \vec{\tau} + \rho \vec{f}$$  \hspace{1cm} (3)
Here, \( \nabla \tau \) is the viscous stress tensor and is the body force per unit mass. The viscous stress tensor for Newtonian fluids is given by \( \nabla \tau \) (in tensor notation):

The Navier-Stokes equation in terms of three scalar components can be described as:

X-component of the momentum equation:

\[
\frac{\partial (\rho u_x)}{\partial x} + \nabla \cdot (\rho u_x u) = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} + \rho f_x \tag{4}
\]

Y-component of the momentum equation:

\[
\frac{\partial (\rho u_y)}{\partial x} + \nabla \cdot (\rho u_y u) = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} + \rho f_y \tag{5}
\]

Z-component of the momentum equation:

\[
\frac{\partial (\rho u_z)}{\partial x} + \nabla \cdot (\rho u_z u) = -\frac{\partial p}{\partial z} + \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} + \rho f_z \tag{6}
\]

The equations (4, 5 and 6) are the Navier-Stokes equations in conservation form. For incompressible flows the second term of the viscous stress tensor given in Eq. (4) is zero due to the incompressibility constraint given in Eq. (2). For constant viscosity, the Navier-Stokes equation for incompressible flows can be written as:

\[
\rho \left[ \frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} \right] = -\nabla p + \mu \nabla^2 \vec{u} + \rho \vec{f} \tag{7}
\]

3.2. Turbulence Model

In this study k-ε turbulence model is used. The k-ε model is one of a family of two-equation models, for which two additional transport equations must be solved in order to compute the Reynolds stresses. (Zero- and one-equation models also exist, but are not commonly used in mixing applications.) It is a robust model, meaning that it is computationally stable, even in the presence of other more complex physics. It is applicable to a wide variety of turbulent flows, and has served the fluid modelling community for many years. It is semi-empirical, based in large part on observations of mostly high Reynolds number flows. The two transport equations (Eq.8 & 9) that need to be solved for this model are for the kinetic energy of turbulence, \( k \), and the rate of dissipation of turbulence, \( \varepsilon \).

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \mu + \frac{\mu_t}{\sigma_k} \right] \frac{\partial k}{\partial x_i} + G_k - \rho \varepsilon \tag{8}
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ \mu + \frac{\mu_t}{\sigma_\varepsilon} \right] \frac{\partial \varepsilon}{\partial x_i} + C_1 \frac{\varepsilon}{k} G_k + C_2 \rho \frac{\varepsilon^2}{k} \tag{9}
\]
The quantities $C_1$, $C_2$, $\sigma$ and $\sigma$ are empirical constants. The quantity $G_t$ appearing in both equations is a generation term for turbulence. It contains products of velocity gradients, and also depends on the turbulent viscosity:

$$G_t = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_i}$$

(10)

$$\mu_t = \rho C_{\mu} \frac{k^2}{\varepsilon}$$

(11)

To summarize the solution process for the $k\cdot\varepsilon$ model, transport equations are solved for the turbulence kinetic energy and dissipation rate. The solutions for $k$ and $\varepsilon$ are used to compute the turbulent viscosity, $\mu_t$, using the results for $\mu_t$ and $k$, the Reynolds stresses can be computed for substitution into the momentum equations. Once the momentum equations have been solved, the new velocity components are used to update the turbulence generation term, $G_t$, and the process is repeated.

3.3. Mesh Generation

The purpose of meshing was to divaricate the entire configurational dominion into small control volumes and then the mathematical equations were employed by making use of the computer numerical calculations. For simulation purpose, the mesh was divided into two main regions, fluid region of impeller and region of impeller rotation and both were establish as a distinct interacting fluid dominion. Fine meshing was employed so as to increase the stability of the model. CFD code fluent was employed for the purpose of numerical simulation. This CFD technique is based on Navier-Stokes equations which comprises of continuity, energy and momentum equations. In all cases, we used tetrahedral elements for meshing. A total grid size of 214200 (r×θ×z: 25×168×51) was used for the full dominion of the tank accuracy of the computation (Fig.3). 3D simulation was done so as to model the flow accurately. For modelling the motion of impeller MRF model was employed. First order upwind discretization scheme is adopted in this study.

![Fig.3: Generated grid for Unbaffled Tank (left) and Baffled Tank (right)](image)

3.4. Boundary conditions

For the unbaffled tanks both Rushton and curve blade the entire computational region was reduced to $60^\circ$, consisting of one blade while for other two vessels which originally consist of six blade and four baffles, the computational region was reduced to $180^\circ$, consisting of 3 blade and 2 baffles. Now there are two types of impeller rotational model multiple reference frame (MRF) and Sliding mesh model. For both the types the entire solution domain is divided into two zones, inner impeller region and outer baffle region. For MRF model, the impeller is considered as rotating reference frame while the outer
baffle region is considered as stationary reference frame. It involves steady state calculations as the solution progresses. In sliding mesh model the impeller region is allowed to slide over the outer region in discrete time step. In this study MRF model is applied for impeller rotation model.

3.5. Convergence criteria
In this study $k$-$\varepsilon$ turbulence model is used for predicting the nature of flow. While normalization and scaling can be done in number of ways, it is the change in the normalized residual that is important in evaluating the rate of convergence. In this study, the simulation is considered to be converged when the residual falls below $10^{-3}$ and steady state of the velocity profile is reached.

4. Numerical Results
The simulated three dimensional mean velocities (radial, tangential and axial) normalized by maximum velocity ($U_{\text{tip}} = ND$ where, $N$ is the impeller speed in revolution per sec and $D$ is the impeller diameter in metre) will be discussed in this section. Velocities were measured at a specific spatial location in the stirred tank and compared for baffled and unbaffled condition for Rushton and Curve blade impeller. The predicted results were also compared with experimental results published in literature.

4.1 Axial Profile of Radial Velocity
The normalized radial velocity ($U_{\text{radial}}/U_{\text{tip}}$) with respect to normalized tank height ($z/H$) comparing between baffled and unbaffled system for Rushton and Curve blade impeller is shown in Fig.4(a&b).

![Fig.4: (a) Radial velocity for Rushton impeller and (b) Radial velocity for Curve blade impeller](image)

In all the four cases, it is found that the radial velocity was maximum in the discharge area of the impeller and then decreases gradually. The radial velocity was found to be highest in baffle tank for both, Rushton and Curve blade impeller. The negative velocity represents that the fluid flow is drawn through the movement of impeller. Specifically in the upper zone it was found that the radial velocity was very low in all the four cases. This proves that the presence of baffle does not impact the radial velocity at the top of tank.

4.2 Axial Profile of Tangential Velocity
Fig.5(a&b) shows the axial profiles of the tangential component of the velocity on the entire height of the tank. In case of Rushton impeller it was found that tangential component of velocity was found to be maximum from $z/H=0.27$ to $z/H=0.4$ whereas in case of Curve blade the tangential velocity was found to be maximum from $z/H=0.3$ to $z/H=0.5$. A recirculation zone was found to be present on both
the sides of impeller in all the four cases. There was sudden decrease of velocity to zero in the unbaffled tank for both the type of impeller which signifies that the movement of fluid was less profound in the unbaffled tank as compare to the baffle tank. Moreover in the unbaffled tank the tangential velocity was found to be most significant than other velocity for both the type of impellers. The tangential velocity was less in baffled tank than unbaffled tank for both the type of impeller which prevents the formation of vortex around the shaft. Hence it was concluded that unlike the radial component the tangential velocity is affected by the presence of baffles.

![Fig.5: (a) Tangential velocity for Rushton impeller and (b) curve blade impeller](image_url)

4.3 Axial Profile of Axial Velocity

Fig.6(a&b) shows the axial profiles of the axial component of the velocity on the height of the tank. There was a great resemblance in all the four cases. A recirculation zone was found to be present on both the sides of impeller. The movement of fluid was found to be more profound in the baffle tank as compare to the unbaffled tank. The increase in the upward axial jet was due to the presence of baffles. At the topmost part of the tank the negative value of the axial velocity indicates that flow is drawn at the shaft to the power of impeller. Thus it was concluded that the presence of baffles intensify the axial jet in both the impellers.

![Fig.6:(a) Axial velocity plot for Rushton impeller and (b) curve blade impeller](image_url)
Fig. 7 shows the distribution of the mean velocity in the r-z plane containing the blades. It is observed that the appearance of a strong centrifugal flow from the blades that reached up to the sidewall of the tank placed in front of the radial jet. In a cylindrical tank, the flow generated by the rotation of the Rushton turbine is very low. The radial jet does not reach the lateral walls. As a result, the presence of the baffles intensified the radial jet which reached the lateral surface which, in turn, caused two axial jets, one up and one down. In the baffled stirred tank, the axial jet was found to be the most significant. This upward jet brought up the recirculation loop extended in the upper area of the tank thereby feeding back to the turbine. We noted a great similarity in the lower area of the second configuration and that of the, presumably because the systems is baffled in the lower zone. Moreover, we noticed a recirculation zone which arose to power the Rushton turbine. But in the upper zone, the upward axial jet dropped sharply in the absence of the baffles in the top of the tank. The recirculation loop in the upper zone was less extensive. Thus, we concluded that the use of baffles on the height of the tank increases the axial 19 jets on either side of the turbine, and furthermore, promotes the circulation of the fluid throughout the volume of the tank. The predicted flows reveal that the Rushton turbine produces a radial flow, which upon impingement on the reactor walls deflects upwards towards the liquid surface. The stream then returns to the stirrer, thus forming a recirculation zone. The principal difference between the flow in an unbaffled stirred tank and that in a baffled tank is the rotation of the liquid, which usually acts as a combined vortex consisting of an inner core of forced-vortex (or solid-body rotation) and an outer region of free-vortex motion resulting in the deformation of the liquid free-surface. In unbaffled agitated vessels, a large vortex is formed because of the free headspace resulting in the deformation of the liquid surface. This has a significant effect on flow and mixing processes.

4.4 Impeller Efficiencies based on Power Consumption

For describing the effectiveness of a mixing system the power consumption is a very significant framework. Fig. 8 represents power efficiency for all the four type of tank configuration.
In this study the efficiency $E$, of the impeller has been calculated by including two flow factors: impeller flow number $N_d$, impeller power number $N_p$ as:

$$E = \frac{N_d^3}{N_p}$$  \hspace{1cm} (12)

$$N_p = \frac{P}{n^3 d^5 \rho}$$  \hspace{1cm} (13)

$$N_d = \frac{Q}{n d^3}$$  \hspace{1cm} (14)

Where, $P$ is the power consumption of the tank, $n$ is the impeller rotational speed, $d$ is the impeller diameter and $\rho$ is the fluid density. For both the type of blades, the power consumption of a baffle tank was found to be greater than the un-baffled tank. Also the efficiency of the baffled tank for both Rushton and Curve blade impeller was found to be better than un-baffled tank. This is due to the presence of low velocity gradient in the baffled tank as compare to the un-baffled tank.

4.5. Comparison with Experimental Results

Fig.9 (a&b) shows the axial profiles of the radial and tangential velocity components in the radial position defined by $r/D = 0.185$ in the baffled stirred tank equipped with the Rushton impeller.

Mean fluid components of an aeration tank should be speculated precisely by a CFD model. However $k-\varepsilon$ turbulence model has been found to under or over project turbulence. In the present work it has
been found that there is a diversion between numerical and experimental data [35] particularly underneath the impeller. In this study the experimental data comprises of 10 data sets from which a continuous graph has been derived. Also any contrast between numerical and experimental data in both this and upcoming sections should be comprehend with the characteristics of the experimental data set [35] in mind i.e. results should be analogous rather than exactly alike.

5. Conclusions
The outcome of numerical evaluation dispensing the effect of vessel configuration on the flow structure and turbulent characteristics has been evaluated. The present work examines the impact of baffle and blade on the power consumption of the impeller. For all the four system it has been found that power number is dependent on the length of baffle. Also the use of baffle increases the circulation and enhances the degree of mixing. The outcome predicted also stipulates that the power consumption and efficiency of tank is influenced by the type of blade used. Although the power consumption of baffle tank was higher than the unbaffled tank, the efficiency of baffled system was better than the efficiency of unbaffled system. Overall the efficiency of the Curve blade impeller was found to better than the other configuration.

References
[1] Lane G L et al 2005 Chem. Engg. Sci. 60 2203
[2] Deglon DA and Meyer CJ 2006 Miner. Engg. 19 1059
[3] Gaubert M A et al 2006 Chem. Engg. Proc. 45 415
[4] Zadghaffari R et al 2009 Computatio. Chem. Engg. 33 1240
[5] Ranade V Vet al 1991 Chem. Engg. Sci. 46 1883
[6] Bridgeman J 2012 Adv. Engg. Soft. 44 54
[7] Gentric C et al 2005 Chem. Engg. Sci. 60 2253
[8] Nagata S 1975 Wiley, New York
[9] Glover G M C and Fitzpatrick J J 2007 Chem. Engg. J. 127 11
[10] Assirelli M et al 2008 Chem. Engg. Sci. 63 35
[11] Aloi L E and Cherry RS 1996 Chem. Engg. Sci. 51(9) 1523
[12] Hekmat D et al 2007 Proc. Biochem. 42 1649
[13] Rousseaux J M et al 2001 Canadian J. Chem. Engg. 79 697
[14] Kagoshima M and Mann R 2006 Chem. Engg. Sci. 61(9) 2852
[15] Tezura S et al 2007 J. Chem. Tech. Biotech. 82 672
[16] Galletti C and Brunazzi E 2008 Chem. Engg. Sci. 63 4494
[17] Yoshida M et al 2008 J. Fluid Sci. Tech. 3 282
[18] Hirata Y et al 2009 Chem. Engg. Res. Des. 87(4) 430
[19] Brucato A et al 2010 Chem. Engg. Sci. 65 3001
[20] Wang B et al 2012 Biotech. Adv. 30 904
[21] Shekhar S M and Jayanti S 2002 Trans. IChemE. 80(A) 482
[22] Alcamo R et al 2005 Chem. Engg. Sci. 60 2303
[23] Cokljat D et al 2006 Prog. Comp. Fluid Dyn. Inter. J. 6(1-3) 168
[24] Nienow A W 1996 Trans. Inst. Chem. Engineers 74(A) 417
[25] Yoshida M et al 1996 Canadian J. Chem. Engg. 74(1) 31
[26] Myers K J et al 1999 Chem. Engg. Res. Des. 77 728
[27] Bakker A 2000 The Online CFM Book
[28] Sardeing R et al 2004 Trans. IChemE382(A9) 1161
[29] Albaek M O et al 2008 Chem. Engg. Sci. 63 5813
[30] Gimun J 2009 Chem. Engg. Sci. 87 437
[31] Ahmed S U et al 2010 J. Biosci. Bioengg. 109(6) 588
[32] Suhaili N et al 2010 J. Appl. Sci. Res. 6(3) 234
[33] Suhaili N et al 2011 UMTAS, 146
[34] Van’t Riet K et al 1976 *Chem. Engg. Res. Des.* **54** 124

[35] Wu H and Patterson G K 1989 *Chem. Engg. Sci.* **44** 2207