

An Overview of Impellers, Velocity Profile and Reactor Design

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Abstract: This paper presents a simulation approach to develop a model for understanding the mixing phenomenon in a stirred vessel. The mixing in the vessel is important for effective chemical reaction, heat transfer, mass transfer and phase homogeneity. In some cases, it is very difficult to obtain experimental information and it takes a long time to collect the necessary data. Such problems can be solved using computational fluid dynamics (CFD) model, which is less time consuming, inexpensive and has the capability to visualize the real system in three dimensions.

As reactor constructions and impeller configurations were identified as the potent variables that could affect the macromixing phenomenon and hydrodynamics, these variables were modelled. Using detailed hydrodynamic modelling of a system, we can optimize the critical parameters and operation limits. Besides the detailed examination of the processes, we can attain better yields and higher quality products.

The results were presented to IOCL in the form of a report. For the implementation of the models COMSOL Multiphysics 3.5 was used.

Keywords: Computational Flow Dynamics, velocity profile, impellers, mixing, stirred vessel

1. Introduction

The stirred vessel is one of the most commonly used devices in the production industry. Chemical reactors are sorted according to the operation (batch, fed-batch, continuous) or the used impeller type (turbine, jet, blade, etc.) or by any similar kind of classification as convenient for the specific industry, the mentioned being majority. The mixing in the vessel is important for effective chemical reaction, heat transfer, mass transfer and phase homogeneity. For the suitable homogeneity, adequate mixing is required which depends on the design and size of the moving parts. Thus, it is an important problem. Static parts attached to a stirred tank (such as baffles) in certain situations may also have a significant effect on mixing phenomena.

A detailed modelling of fluid dynamics will help in determining the regimes of

operation and hence in estimating the efficiency of the operating system. The involved processes can be analysed to optimize the products of a technology, through defining the model with adequate parameters.

Reactors are always important parts of any working industry, and for a detailed study using several parameters many readings are to be taken and the system has to be observed for all adversities of environment to correct for any skewness of values. As such huge amount of required data, it takes a long time to collect enough to build a model. In some cases, also it is difficult to obtain experimental information also. Pilot plant experiments can be considered as an option, but this conventional method has been left far behind by the advent of Computational Fluid Dynamics (CFD) models owing to its main advantage examining the real system in three dimensions along with option for scaling. A validated CFD model can support design, research and development, optimization, scale up or other complex engineering tasks, such as polymerization and crystallization operations.

In our research work, COMSOL Multiphysics 3.5 has been used, in which Different reactors with varying impeller configurations have been modelled to achieve a better understanding of mixing and hydrodynamics in a stirred tank. Velocity profile and homogeneity of the system were studied. The reactor constructions were flat bottom and ellipsoid bottom tank with different types of impellers: T shaped impellers, rotating disc, three-bladed impeller, four-bladed impeller and pitched blade impellers [Figure-1]. Each reactor configuration was simulated at different revolution speeds such as 10, 20, 50 and 100 RPM. With this detailed modelling, the ideal parameters were computed for reactor design.

The achieved results are shown in three dimensional animations, and streamline diagrams. Background study involves the governing equations which are needed to describe mixed systems and are mentioned in the section that follows.

2. Governing Equations

The flow is described by the Navier-Stokes equations having the local changes term, the convective term, stress term, and the body forces term (F)

$$\rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla)u = \nabla \cdot \left[-pI + \eta \left(\nabla u + (\nabla u)^T \right) \right] + F$$

$$\nabla \cdot u = 0$$

The next equation is the continuity equation, describing the conservation of mass.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0$$

Two models were used to describe turbulence modeling variable k-ε models and Reynolds averaged Navier-Stokes equations. The k-ε models use a modified Navier-Stokes equation, calculating the velocity field by using turbulence viscosity. In the Reynolds averaged Navier-Stokes equation the stresses are calculated as average stresses to lower the need of computation. Equation expresses the stress tensor (P_k)

In these equations, **u** denotes for velocity (m/s), the density (kg/m³), the dynamic viscosity (Pa.s), and p the pressure (Pa). For a stationary, axisymmetric flow the equations reduce to

$$\rho \left(u \frac{\partial u}{\partial r} - \frac{v^2}{r} + w \frac{\partial u}{\partial z} \right) + \frac{\partial p}{\partial r} = \eta \left(\frac{1}{r} \frac{d}{dr} \left(r \frac{\partial u}{\partial r} \right) - \frac{u}{r^2} + \frac{\partial^2 u}{\partial z^2} \right) + F_r$$

$$\rho \left(u \frac{\partial v}{\partial r} + \frac{uv}{r} + w \frac{\partial v}{\partial z} \right) = \eta \left(\frac{1}{r} \frac{d}{dr} \left(r \frac{\partial v}{\partial r} \right) - \frac{v}{r^2} + \frac{\partial^2 v}{\partial z^2} \right) + F_\theta$$

$$\rho \left(u \frac{\partial w}{\partial r} + w \frac{\partial w}{\partial z} \right) + \frac{\partial p}{\partial z} = \eta \left(\frac{1}{r} \frac{d}{dr} \left(r \frac{\partial w}{\partial r} \right) + \frac{\partial^2 w}{\partial z^2} \right) + F_z$$

To describe turbulent flow in the reactor the model uses the k-ε model, for which the momentum transport and continuity equations are:

$$\rho \frac{\partial U}{\partial t} - \nabla \cdot \left[\left(\eta + \rho \frac{C_\mu k^2}{\sigma_k \varepsilon} \right) \cdot \left(\nabla U + (\nabla U)^T \right) \right] + \rho U \cdot \nabla U + \nabla P = 0$$

$$\nabla \cdot U = 0$$

Where, ρ denotes the fluid's density (kg/m³), **U** represents the average velocity (m/s), η is the dynamic viscosity (kg/(m.s)), P equals the pressure (Pa), k refers to the turbulence energy (m²/s²), ε is the dissipation rate of turbulent kinetic energy (m²/s³) and is a model constant.

3. Modelling and method

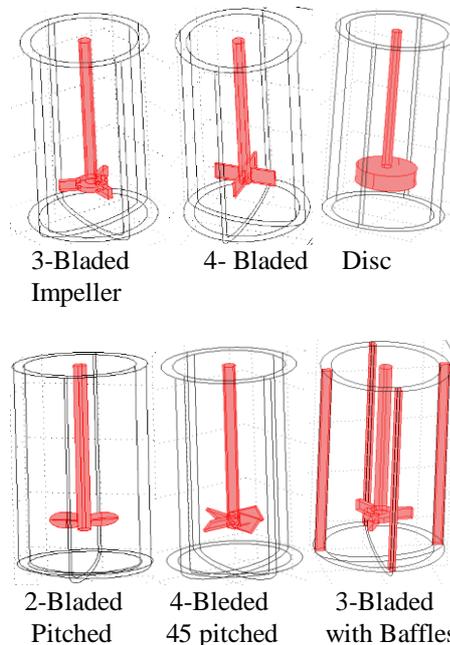
Single phase fluids were examined in laminar and turbulent regimes for modelling a stirred tank reactor. We used COMSOL Multiphysics 3.5 to implement the models.

The fluid properties are described by mainly three parameters: revolution speed, density and viscosity. The density used is the density of the water, and the dynamic viscosity is equal to the value of the viscosity, took from the model library built-in example.

Table 1 Model Parameter used

rpm	Revolution speed	20,50,100	1/min
rho	Density	1000	Kg/m ³
eta	Viscosity	0.01	Kg/(m.s)

For every impeller a 3D geometry was drawn and exported to the different tank geometries. Figure 1 shows the different impeller geometries.



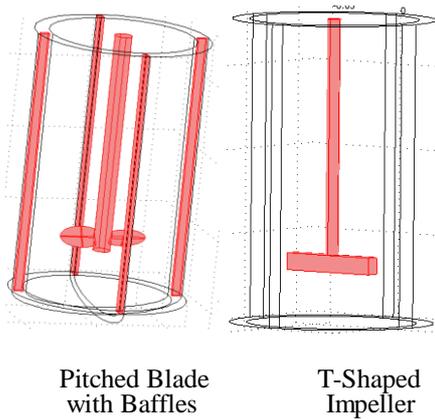


Figure 1 The used impellers

The results are shown for a model obtained from model navigator using chemical engineering module. The designed reactor is an ellipsoid bottom tank with a 4-bladed impeller. The geometry was created in COMSOL Multiphysics 3.5 manually, using geometry modelling. The stirred vessel was created from cylindrical and ellipsoid shapes. Using identity pair, the designed geometry (reactor vessel and impeller) was assembled. Identity pairs were used to join the rotating part (impeller) to the fixed part (reactor vessel). We choose chemical engineering module with rotating machinery from COMSOL Multiphysics for the moving mesh model. The investigated model has two subdomains: the outer subdomain is fixed, and the inner subdomain rotates. The identity pair describes the connection between the two subdomains. Table 2 contains the geometry parameters described the given model, and Figure 2 shows the finalized geometry.

Table 2 Geometry parameters

Inner subdomain diameter	1	m
Outer subdomain diameter	1.2	m
Reactor height	1.8	m
Impeller diameter	0.33	m
Impeller height	1.5	m
Impeller bottom distance	0.15	m

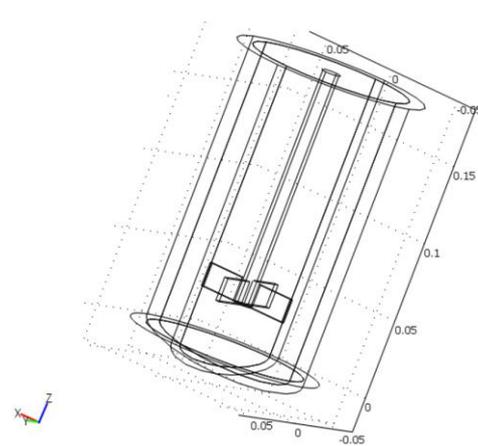


Figure 2 The finalized geometry

The fluid properties are designed by user itself. In Physics menu user defined the wall boundary and the outer boundaries conditions except for the upper two boundaries, those were symmetry boundaries. The rotating domains: the inner subdomain and rotating wall have the similar boundary conditions as the impeller have. Every simulation had done for three different values of rotational speed with counter clockwise direction having positive angular velocity. Identity pair defined the flow between the outer and inner subdomain. One of the points of the upper edge of the reactor was fixed as a pressure point constraint. In every case, put initial values of the velocity in every direction zero.

A user defined mesh with tetrahedral elements was used in every simulation. In this particular case coarse mesh is used. Figure 3 shows the meshed geometry.

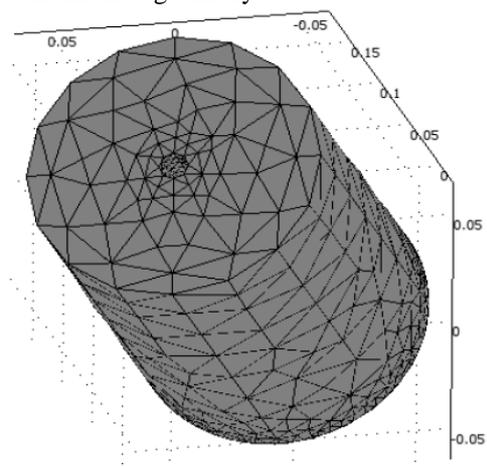


Figure 3 The meshed geometry

The results are shown as slice diagrams showing the velocity field in the vessel geometry, and streamline diagrams. Animations were created from the slice

diagrams to visualize dynamical behaviour of the system.

4. Results and discussion

The slice plot is the type of post processing. In Figure 4 five parallel vertical slices are implemented through the whole diameter of the reactor, which shows the results of the dynamic simulation, the velocity field in the case of 4-bladed turbine impeller. The revolution speed is 100 1/min. The figure shows, that the fluid velocity is higher near the impeller than near the wall.

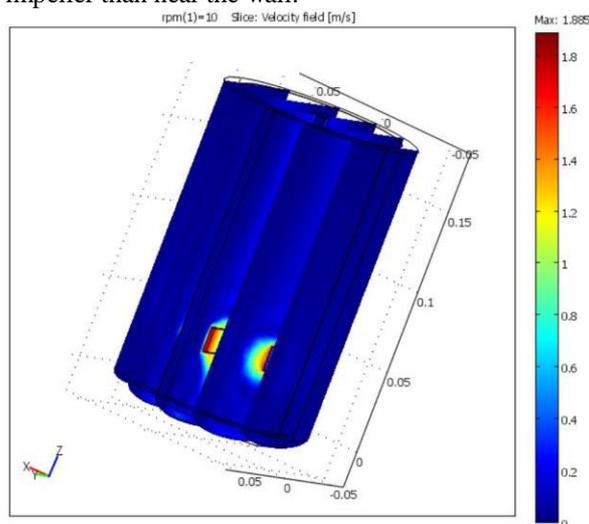


Figure 4 The simulation results of the stirred tank with a 4-bladed impeller. (100 1/min)

Figure 5 shows the streamline plot of the vorticity affects mixing phenomena. The streamline plot shows, that the reactor is well mixed. Baffles can be used to achieve a adequate mixing in stirred vessel when vorticity is formed.

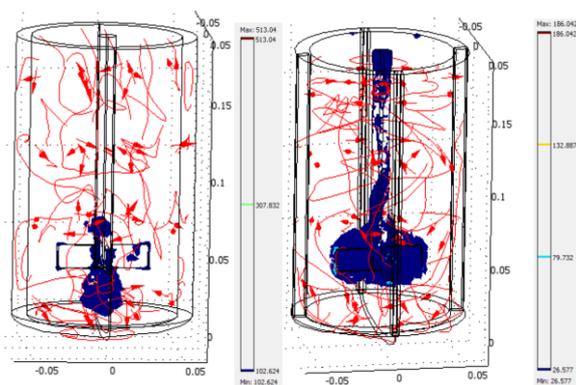


Figure 5 : The streamline plot of vorticity with and without baffles
Maximum vorticity of 4-bladed impeller with and without baffles is 513.04 and 186 respectively. Hence, vorticity is reduced by

introducing baffles when pitch is not presented for 4-bladed impeller

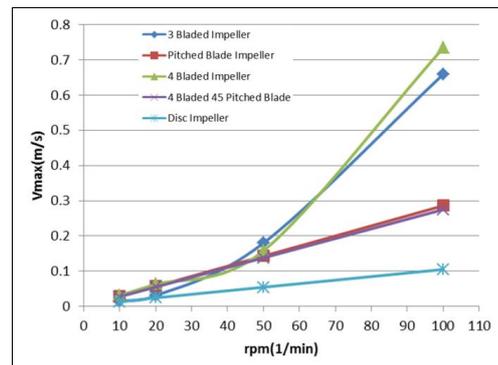


Figure 6: The velocity profile for different type of impellers

Figure 6 shows velocity profile for different impellers at time 60s by stationary solver. The graph shows, that average velocity of fluid in stirred vessel increases with rotational speed and also shows that the average velocity for 4-bladed impeller is greater among three bladed impeller, 2-bladed pitched blade impeller, 4-bladed impeller, 4 bladed 45° pitched blade impeller and disc impeller for higher revolution speed

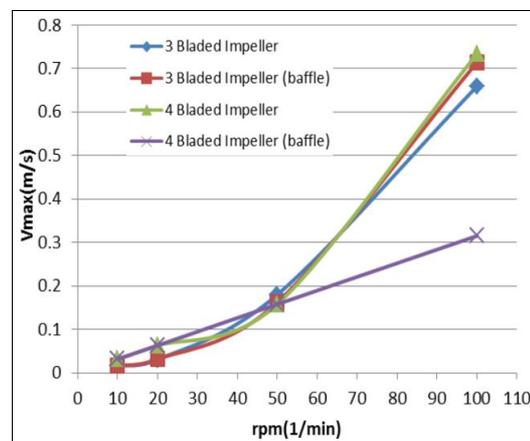


Figure 7: The velocity profile for 3-bladed and 4-bladed impellers with and without baffles

Figure 7 shows comparison of velocities between 3-bladed and 4-bladed impellers with and without baffles at time $t = 60$ sec by stationary solver. It's evident that the average velocity of impellers with baffles is less than the one without baffles and the difference increases with rotational speed. Hence, baffles helps in preventing vortex formation.

The above graph shows, that the 4-bladed impeller has greater velocity than 3-bladed impeller but in case of impellers with baffle the 3-bladed impeller has greater velocity than 4-bladed impeller.

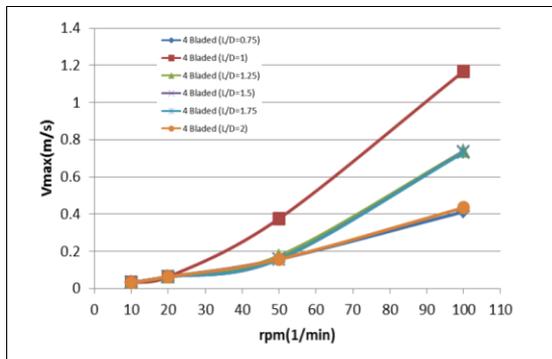


Figure 8: The velocity profile for different reactor geometry.

Reactors always play an important role in any working industry. Designing of reactor affects reaction rate as well as installation cost. To make industry more economically profitable, optimized reactor parameters are required.

Figure 8 shows velocity profile of 4-bladed impeller for different reactor geometry at time 60 sec by stationary solver. It's evident that velocity of 4-bladed impeller is optimum at $L/D = 1$ for higher revolution speed.

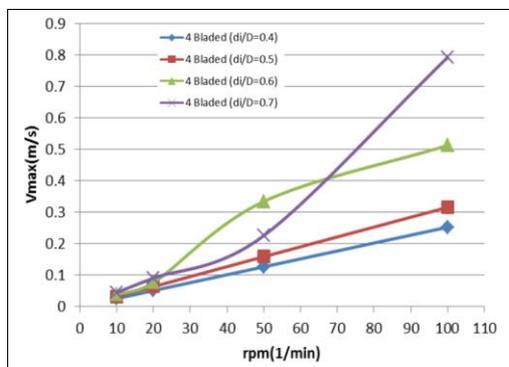


Figure 9: The velocity profile for different ratio of impeller to reactor diameter

Impellers are used in reactor for effective mixing to produce the desired effect in the least amount of time. Here, different reactors with varying impeller configurations have been modeled to achieve a better understanding of mixing and hydrodynamics in a stirred tank.

The above graph shows velocity profile of 4-bladed impeller for different ratios of the impeller diameter to the reactor diameter at time 60s by stationary solver. It's evident that velocity for 4-bladed impeller is optimum at $di/D = 0.6$ and $di/D = 0.7$ for lower revolution speed and higher revolution speed respectively.

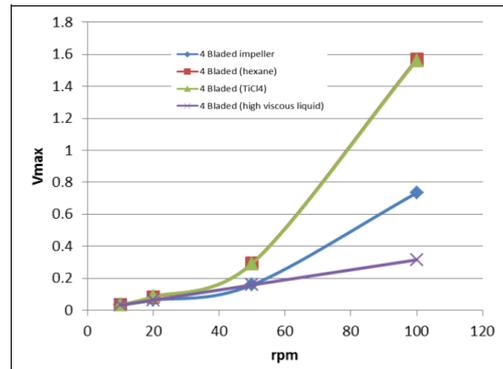


Figure 10: The velocity profile for different fluids

The fluid properties like density and viscosity also affect the rate of mixing. The average velocity decreases as viscosity of fluid increases.

Figure 10 shows velocity profile of 4-bladed impeller for different fluids at time 60s by stationary solver. It is obvious that velocity for hexane and $TiCl_4$ (less viscous fluid) is greater than the water and high viscous fluid.

5. Conclusions

Velocity profile and mixing in stirred vessel has been investigated using computational fluid dynamics (CFD). The purpose was to understand the effect of reactor geometry, impeller configuration, rotation speed, baffle and fluid properties (density and viscosity) on the mixing phenomenon. The results are shown in the form of slice diagrams, streamline plots and graphs. In future, one can do the same simulation for higher revolution speed, multi-impeller systems and continuous systems.

6. References

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7. Acknowledgements

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8. Appendix

Table 1 : Notation

Variable	Description	Unit
ρ	density	[kg/m ³]
μ	viscosity	[Pas]
μ_t	turbulent viscosity	[Pas]
k	turbulent kinetic energy	[m ² /s ³]
ε	energy dissipation rate	[m ² /s ²]
u	velocity vector	[m/s]
ω	angular velocity	[rad/s]
r	radius	[m]
t	Time	[s]
∇	nambla	
F	force vector	N
P	pressure	Pa

Table 2: The velocity profile for different reactor and impeller configuration

10 rpm										
Impeller	di/D				L/D					
	0.4	0.5	0.6	0.7	0.75	1	1.25	1.5	1.75	2
3-bladed	0.0104	0.0155	0.02	0.0202	0.0205	0.0162	0.0198	0.0155	0.0147	0.0118
4-bladed	0.0252	0.0315	0.0378	0.0444	0.0315	0.0315	0.0315	0.0315	0.0315	0.0315
4-bladed 45°pitch	0.0179	0.0278	0.0313	0.0378	0.0294	0.0286	0.0283	0.0278	0.0287	0.0254
20 rpm										
Impeller	di/D				L/D					
	0.4	0.5	0.6	0.7	0.75	1	1.25	1.5	1.75	2
3-bladed	0.0224	0.0304	0.0414	0.0422	0.0403	0.0318	0.04	0.0304	0.0272	0.0228
4-bladed	0.0504	0.063	0.0757	0.0903	0.063	0.063	0.063	0.063	0.063	0.063
4-bladed 45°pitch	0.0344	0.0551	0.124	0.26	0.0579	0.0528	0.0562	0.0551	0.057	0.0494
50 rpm										
Impeller	di/D				L/D					
	0.4	0.5	0.6	0.7	0.75	1	1.25	1.5	1.75	2
3-bladed	0.0479	0.18	0.252	0.181	0.099	0.169	0.139	0.18	0.171	0.0672
4-bladed	0.126	0.158	0.334	0.225	0.158	0.376	0.176	0.158	0.158	0.158
4-bladed 45°pitch	0.0805	0.138	0.407	0.348	0.144	0.126	0.14	0.138	0.141	0.121
100 rpm										
Impeller	di/D				L/D					
	0.4	0.5	0.6	0.7	0.75	1	1.25	1.5	1.75	2
3-bladed	0.177	0.659	0.73	0.686	0.223	0.768	0.499	0.659	0.773	0.28
4-bladed	0.252	0.315	0.512	0.792	0.413	1.169	0.739	0.734	0.732	0.435
4-bladed 45°pitch	0.172	0.275	0.31	0.375	0.495	0.597	0.279	0.275	0.281	0.239

In table 2, shows the average velocity for different reactor and impeller configurations. From the table one can easily conclude the optimized reactor and impeller configuration for stirred vessel using in industry. Using table 2, for a given reactor size, one can easily suggest which impeller is best for the given reactor design and vice-versa.