Investigations on Hydrodynamic in Stirred Vessels for Educational Purposes

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Abstract: Engineering problem solving such as process design, process optimization, safety analysis, etc.; relies widely on mathematical models of the process. By detailed hydrodynamic modeling of a system the critical parameters and operation limits can be determined. Beside the detailed examination of the processes we can attain better yields and higher quality products.

To understanding the macromixing phenomenon, and hydrodynamics in a stirred tank different reactor constructions and impeller configurations were modeled. All of the results were presented in an open access website in the form of animations, and pictures. For the implementation of the models COMSOL Multiphysics 4.1 was used. The website is intended to support high school education and fluid dynamic studies in universities too.

Keywords: Computational Fluid Dynamics, stirred vessel, reactor engineering education, macromixing

1. Introduction

The stirred vessel is one of the most widely used devices in the industry. There are several way to sort chemical reactors, for example by operation (batch, fed-batch, continuous), or by the used impeller type (turbine, jet, blade, etc.)[1]. The mixing system of the vessel is always an important aspect of design, because the involved processes (chemical reaction, heat or component transport) need adequate mixing, and phase homogeneity. For the suitable homogeneity the design and size of the moving parts is also an important problem. In certain situations attachment of static parts to a stirred tank (such as baffles) may have a significant effect too [2].

With the detailed modeling of fluid dynamics, operating regimes can be determined, and the system can be operated with the expected efficiency. With the analysis of the involved processes there is a possibility to optimize the products of a technology, with defining the adequate model parameters.

Industrial reactors are almost always important parts of a working technology, therefore in some cases it is difficult to obtain experimental information, and it takes a long time to collect enough data to build a model. One of the solutions can be the pilot plant experiments, or using Computational Fluid Dynamics (CFD) models. The main advantage of a CFD model is the capability of examining the real system in three dimensions [3]. A validated CFD model can support design, research and development, optimization, scale up or other complex engineering tasks, such as polymerization and crystallization operations [4, 5, 6, 7].

In our research several different reactor constructions and impeller configurations were modeled to achieve deeper understanding on mixing, and hydrodynamics in a stirred tank. The reactor constructions were flat bottom, spherical and ellipsoid bottom tank with different type of impellers: two types of turbine impellers, two types of blade and anchor impellers. For every geometry a dynamic model was implemented to examine the reactor startup, and the operation of the vessel. Every reactor configuration was simulated at three different revolution speeds 20, 50 and 100 1/min.

The achieved results are shown in three dimensional animations, and streamline diagrams, and are published via YouTube and an open access website. The website also contains an introduction about mixing, Computational Fluid Dynamics, and COMSOL Multiphysics.

The primary goal of developed website is to introduce mixing, demonstrate the governing equations which are needed to describe mixed systems, and present CFD simulation examples.

2. Governing Equations

To calculate the developed flow field in the laminar regimes of the investigated reactors Navier-Stokes equation was applied.

The first governing equation in the laminar models is the Navier-Stokes equations (2.1), containing the local changes term, the convective term, the stress terms, and the body forces term (F).

$$\rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla)u =$$
$$= \nabla \cdot \left[-pI + \mu\left(\nabla u + (\nabla u)^T\right) - \frac{2}{3}\mu(\nabla u)I \right] + F \quad (2.1)$$

The next equation is the continuity equation (2.2), describing the conservation of mass.

$$\frac{\partial p}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (2.2)$$

The last governing equation of the laminar models describes the rotation of the system (2.3). The (2.3) equation was implemented in turbulent cases too.

$$dx = dx(r_{bp}, \omega, t) \quad (2.3)$$

For turbulence modeling two variable k-ε models and Reynolds averaged Navier-Stokes equations are used. The k-ε models uses a modified Navier-Stokes equation (2.4) calculating the velocity field by using turbulence viscosity (2.7). In the Reynolds averaged Navier-Stokes equation the stresses are calculated as average stresses to lower the need of computation. Equation (2.8) expresses the stress tensor (P_k)

$$\rho \frac{\partial u}{\partial t} + \rho(u \cdot \nabla)u = \nabla \cdot \left[-pI + \right.$$
$$+ (\mu + \mu_T)\left(\nabla u + (\nabla u)^T\right) -$$
$$\left. - \frac{2}{3}(\mu + \mu_T)(\nabla u)I - \frac{2}{3}\rho kI \right] + F \quad (2.4)$$

The term k refers to turbulent kinetic energy, and describe the movement of large eddies (2.5).

$$\rho \frac{\partial k}{\partial t} + \rho(u \cdot \nabla)k = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_k}\right)\nabla k \right] + \quad (2.5)$$
$$+ P_k - \rho\varepsilon$$

The term ε refers to turbulent energy dissipation, and describe the energy dissipation of the small eddies (2.6). Turbulence viscosity is expressed using the turbulent kinetic energy and the turbulent energy dissipation (2.7).

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho(u \cdot \nabla)\varepsilon = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_e}\right)\nabla\varepsilon \right] + \quad (2.6)$$
$$+ C_{\varepsilon 1}\frac{\varepsilon}{k}P_k - C_{\varepsilon 2}\rho\frac{\varepsilon^2}{k}$$

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon} \quad (2.7)$$

$$P_k = \mu_T \left[\nabla u : \left(\nabla u + (\nabla u)^T\right) - \frac{2}{3}(\nabla \cdot u)^2 \right] - \quad (2.8)$$
$$- \frac{2}{3}\rho k\nabla \cdot u$$

3. Modeling and method

3.1 Model generation using COMSOL Multiphysics

Two models were used based on the laminar or turbulent model for modeling a stirred tank. Single phase fluids were examined; laminar and turbulent rotating machinery models were implemented from COMSOL Multiphysics. Three model parameters were used to describe revolution speed and fluid properties. The density is the density of the water, and the dynamic viscosity is equal to the value of the viscosity from the model library built-in example.

Table 1 shows the model parameters.

Table 1 Model Parameters

rpm	Revolution speed	20,50,100	1/min
eta	Viscosity	1	Pas
rho	Density	1000	kg/m^3

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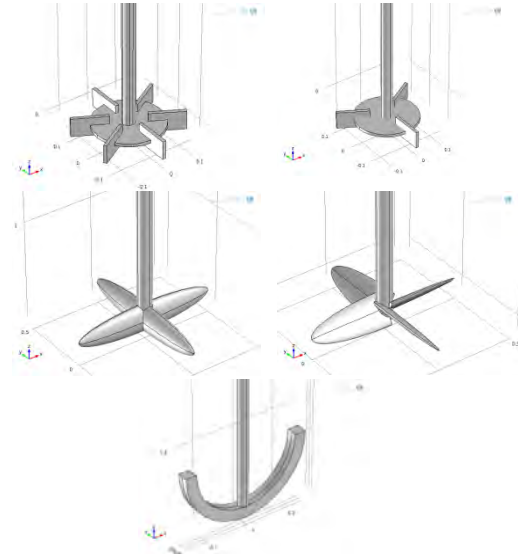

Figure 1 The used impellers

In the next section an example is show from model building obtain results. The investigated reactor is an ellipsoid bottom tank with a three bladed turbine impeller. The full

geometry was created in COMSOL Multiphysics user interface, using geometry drawing and Boolean operations. The reactor vessel was created from cylindrical and ellipsoid shapes. At the end of geometry implementation the full geometry (reactor vessel, and impeller) are assembled by using identity pairs. Identity pairs were used to model the joint surface of the rotating, and fixed parts. COMSOL Multiphysics rotating machinery models use the moving mesh model. The outer subdomain is fixed, and the inner subdomain rotates. The identity pair describes the connection between the two subdomains. Table 2 contains the vessel and impeller parameters, and Figure 2 shows the finalized geometry.

Table 2 Geometry parameters

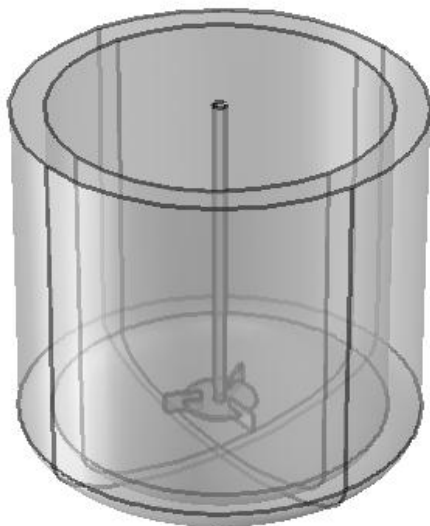| Inner subdomain diameter	1	m
Outer subdomain diameter	1.2	m
Reactor height	1.2	m
Impeller diameter	0.33	m
Shaft diameter	0.1	m
Impeller bottom distance	0.2	m

Figure 2 The finalized geometry

The material was user defined based on the model parameters discussed before. Wall boundary was defined all of the outer boundaries except for the upper two boundaries, those were symmetry boundaries. The rotating domain is the inner subdomain, and rotating wall boundary was defined all of the impeller and shaft boundaries. The revolution speed was one of the previously defined three values and the rotational direction was a positive angular velocity in every case (counterclockwise). Flow continuity was defined for the identity pair between the outer and inner subdomain. One of the points of the upper edge of the reactor was fixed as a pressure point constraint. The initial values of the velocity in every direction were zero, because the reactor startup was examined too.

In every case a user defined mesh was used with tetrahedral elements, in this particular case the mesh contain 103801 elements. Figure 3 shows the meshed geometry.

Figure 3 The meshed geometry

The number of degrees of freedom was 738549 in this simulation. The computation time is strongly depends on the revolution speed. At low revolution speeds (20 and 50 1/min) an FGMRES iterative solver was used with Incomplete LU preconditioner. For 100 1/min revolution speed a direct solver (PARDISO) was used. Each study was time dependent from 0 to 10 s with 0.1 s step size.

The results are shown as slice diagrams showing the velocity field in the vessel geometry, and streamline diagrams. From the slice diagrams animations were created to examine the reactor startup and the dynamical behavior of the system.

3.2 Contents of the website

The first section of the website contains useful information about mixing, dimensionless numbers related to mixing, and different models can use to model mixing. The second part of this section is an introduction to Computational Fluid Dynamics, and COMSOL Multiphysics.

The second section contains the results of the simulation examples. The first step is to select which cases we want to examine, by using a query form. There are multiple parameters which can be given to define the desired configurations.

The vessel geometry
- flat bottom;
- round bottom;
- ellipsoid bottom.

Impeller geometry – must choose one
- six-bladed turbine impeller;
- three-bladed turbine impeller
- blade impeller;
- anchor impeller;

Rotational speed
- 20 1/min;
- 50 1/min;
- 100 1/min.

After filling the form the next page contains all the chosen possibilities, with streamline results. By clicking the pictures an animation will be started which shows the result of dynamical simulationThe results of the mechanical impellers are shown in the form of dynamic simulation. For video sharing a YouTube channel was used [8, 9]. The turbulent and the 45° blade impeller examples are acessible via the YouTube channel. Figure 4 shows the YouTube channel.
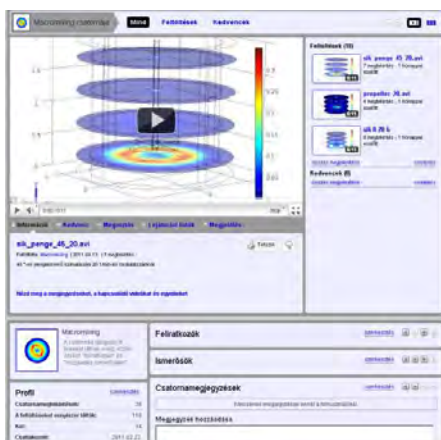

Figure 4 The YouTube channel

The website is available in an open access way. Student can use the site to examine the macro mixing phenomenon, and the reactor startup. A YouTube channel (Macromixing) is used to upload the animations.

4. Results and discussion

The first post processing type was the slice plot. Five parallel xy slices are implemented through the whole height of the reactor. Figure 5 shows the results of the dynamic simulation, the velocity field in a slice plot in the case of three-bladed turbine impeller. The revolution speed is 20 1/min in the upper picture, 50 1/min in the lower picture.
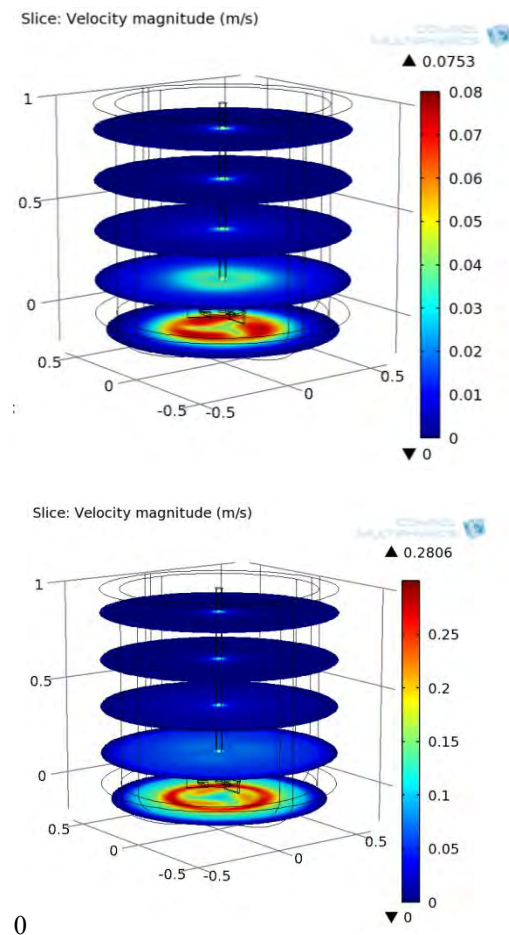

Figure 5 The results of the slice plot in a ellipsoid bottom reactor with a three-bladed turbine impeller (20 1/min, 50 1/min)

The figure shows, that the velocity near the impeller blades is higher, than near the wall, and in the 50 1/min case the average velocity is higher, than in the 20 1/min case. Figure 5 shows the streamline plot of the reactor.
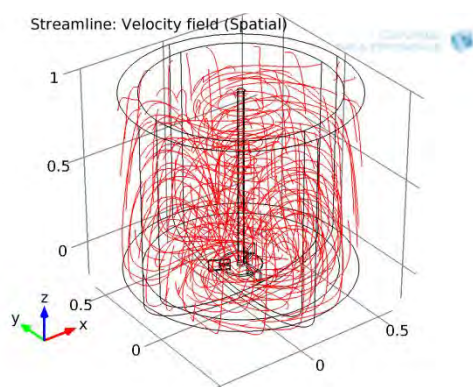
Figure 6 The streamline plot of the reactor Revolution speed [20 1/min]

The streamline plot shows, that the reactor is well mixed. The three-bladed turbine impeller is well enough to achieve adequate mixing in this case. However the exact velocity data cannot extracted from this plot.

5. Conclusions

Different stirred reactors were simulated with different reactor configurations, and impeller geometries. The results were shown in the form of slice diagrams, and streamline plots. From the slice diagrams animations were created

The achieved results were uploaded to an open access website, containing teaching material about mixing, and Computational Fluid Dynamics. The simulation results are shown in animations. The site can support high schools, and even university education.

6. References

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7. Acknowledgements

8. Appendix

Table 3: Notation

Variable	Description	Unit
ρ	density	[kg/m^3]
u	velocity vector	[m/s]
μ	viscosity	[Pas]
μ_t	turbulent viscosity	[Pas]
k	turbulent kinetic energy	[m2/s3]
ε	energy dissipation rate	[m^2/s^2]
C_ε	constant	1.3
$C_{\varepsilon1}$	constant	1.44
$C_{\varepsilon2}$	constant	1.92
C_μ	constant	0.09
σ_k, σ_ε	constant	1
r_{bp}	radius	[m]
I	identity matrix	
ω	angular velocity	[rad/s]
t	time	[s]
∇	nambla	
F	force vector	N
P_k	stress tensor	