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CFD simulation of the agitated batch

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Annotation - English: The literature research and a designed model of agitated batch in software ANSYS are presented in this thesis. Moreover, simulated the fluid flow in the agitated batch by using LES method. After simulation, I compared the simulation results with experimental data in the literature. In addition, the model were optimized by increasing the mesh elements and simulated once more. Simulation results from both models were evaluated in terms of the predicted flow field, flow number, power number, and velocity profiles.

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Declaration

I confirm that the Master thesis was disposed by myself and independently, under leading of my thesis supervisor. All sources of the documents and literature are stated.

In Prague

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1. INTRODUCTION

Mixing of multi component fluids in chemical and industrial applications, often counts as an important part of each processes. Even though laminar is hard for engineers to analyze, the challenge becomes much bigger when it comes to turbulent flows. The nature of turbulent is caustic and complex. Many methods have been developed both analytical and numerical for analyzing turbulent flow in mixer. As it appeared analytical or manually methods of analyzing turbulent regime, are often time consuming and expensive. Numerical methods are relative cheap. As a result of numerical methods one is able to obtain a device model which will help to design mixer and estimate power consumption, velocity profile and pressure distribution in the mixing vessel.

Among many developed turbulent models, each of them have their advantages and disadvantages. Some methods are more precise but more time and resource consuming. In addition, some methods are suitable only for few applications. In this work, we will go through basic theory of each the turbulence models and general theory of mixing and experimental methods. The application so called large eddy simulation (LES) has been used to investigate stirred tank in this thesis. We will be using the software Ansys (fluent). The model of the stirred tank will be created in Solid Works. After creation of the model, the model will be transferred to Ansys to be meshed and simulated. Thereafter we will be able to predict the main parameters for the design such power number, flow number velocity profile and so on. The simulated parameters will be compared with results from experimental data for how good they match each other. In the end, the results and accuracy of the model will be discussed.

Other main task of the thesis is to optimize the mesh of the model. As we know mesh quality effects significantly the result of the simulation. The smaller size of the mesh, the more precise we might get, but as we increase mesh element number we increase calculation time.

Vessels types and design

Mixing in agitated tanks can be done in continuous or batch reactor. Proper mixing result is important for reducing investment and operating costs, providing high yields when mass transfer is limiting, and thus enhancing effectiveness. Processing with mechanical or chemical mixers follows under either laminar or turbulent flow conditions, and it has

connection with impeller Reynolds number Re . [1]

An optimum method to designing the mixing systems consists of following steps

- 1- Define mixing requirements such as blending quality, drop size, mass flow rate.
- 2- It is important to choose a proper impeller that depends on mixing requirements and type of fluid in the mixing.
- 3- Then one is able to determine the correct number of impellers, dimension of the impeller, determine mixer speed and estimate energy requirements.
- 4- Baffles: based in chosen flow arrays.
- 5- Determine dimensions of mechanical components, such as shaft diameter, impeller blade, baffles and supports, bearings, seals, etc. [1]

Geometry of stirred tanks

A common stirred tank consists of a vessel equipped with a rotating mixer. The vessel is often constructed in vertical cylindrical tank. Nonstandard vessels such as those with square or rectangular cross section, or horizontal cylinder vessel is sometimes used. The rotating mixer consists of many components, an impeller, shaft, shaft seal, gearbox, and a motor drive. Wall baffles are usually installed for transitional and turbulent mixing to check solid body rotation and cause axial mixing between the top and bottom of the tank. In high and big tanks, the mixer may be installed from the bottom to decrease the shaft length and order mechanical stability. [1]

Wall baffles

Baffles are generally used in turbulent mixing applications, with the exception of in severe fouling systems, which require fouling systems that require often cleaning of tank internals. For laminar mixing of viscous fluid, baffles are not required.

Tank Bottoms

The stirred vessel are often cylindrical tank with a flat or dished bottom. Dished bottom head can be 1:2 ellipsoidal, ASME dish, or hemispherical. The flow patterns below the impeller can be changed with different head and results in different mixing productivities.

Types of Impeller

The typical impellers used in turbulent mixing are separated into diverse general classes, based on flow regime, applications, and geometries specifications. The classifications also expressed application types for which impellers are used.

Impeller classes and specific types [1]

Table 1. Impeller classes and types

Axial flow	Propeller, pitched blade turbine, hydrofoils.
Radial flow	Flat-Blade impeller, disk turbine, hollow-blade turbine (Smith).
High shear	Cowles, disc, bar, pointed blade impeller.
Specialty	Retreat curve impeller, sweptback impeller, spring impeller, glass-lined turbines.
Up/down	Disk, plate, circles.

Draft tubes

A draft tube is a rounded tube mounted inside the vessel. Axial flow impellers placed inside a draft tube are used efficient “top to bottom” circulation pattern, which is significant flow flow-controlled process. Draft tubes decrease the ordinary deviations in process variables such as concentration, density and viscosity.

2. CHARACTERISTICS OF A STIRRED TANK

Power and power consumption

One of the most important characteristic of a stirred tank mixer is Power consumption, it is directly effecting price of the device. Other characteristics such as flow field around the impeller, shear stress and pressure profile are also necessary to be calculated to design a stirred tank mixer. Primarily, we calculate total required torque to rotate the impeller, and then we will be able to estimate the needed power consumption of the mixer. The torque on each blade numerically is defined as [2]:

$$\Gamma = \sum_i (\Delta p)_i A_i r_i \quad \text{Equation (1)}$$

i is the summation of cells according to each blade. Δp is pressure difference around the impeller at the surface element i and r_i is the radial distance from the axis of the shaft on which the impeller is mounted. For a steady rotation speed of N revolution per second of an impeller to have m blades, the power required is obtained by

$$P = 2\pi N m \Gamma \quad \text{Equation (2)}$$

Then dimensionless characteristics so called power number is calculated.

$$P_0 = \frac{P}{D^5 * \rho * N^3} \quad \text{Equation (3)}$$

Where P_0 is power number, D is the outer diameter of the impeller and ρ is the density of the liquid. An alternative method of calculating the power is to carry out a stream of the turbulent energy dissipation rate, ε , over the whole tank. In the context of LES, the total dissipation $\langle \varepsilon \rangle$ was the sum of the dissipation of the sub-grid scales, $\langle \varepsilon_{sgs} \rangle$, and the viscous dissipation connected with the decided scales, $\langle \varepsilon_l \rangle$, finally the total dissipation is define as:

$$\langle \varepsilon \rangle = \langle 2(v_t + v)|\bar{S}|^2 \rangle$$

where $\langle \rangle$ represents a numerical average over the whole tank. Lastly, the power was completed by multiplying $\langle \varepsilon \rangle$ in the tank volume.

The graph below represent power characteristics of high-speed impellers operated in baffled vessel, 1 – six-blade turbine with disk (Rushton turbine) (CVS 69 1021), 2 – six-blade open turbine, 3 – pitched six-blade turbine with pitch angle 45 (CVS 69 1020), 4 – Pitched three-blade turbine with pitch angle 45° (CVS 69 1025.3), 5 – propeller (CVS 60 1019), 6a,b – high shear stress impeller. [3]

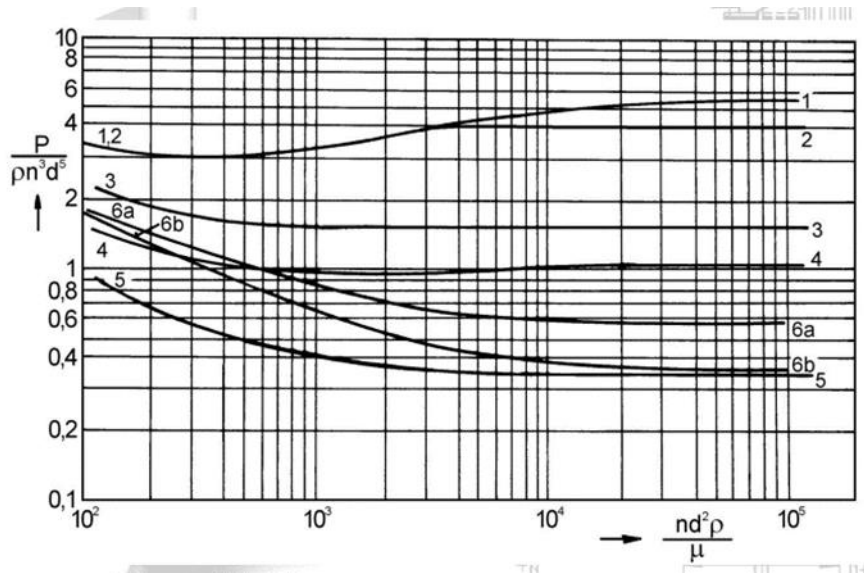


Figure 1. Power number against Reynolds number (log-log scale)

Flow number

The flow number is a number of the pumping capacity of an impeller. Many methods has been devolved for pumping capacity, but the flow number is often used. It is defined as: [1].

$$N_Q = \frac{Q}{N * D^3} \quad \text{Equation (4)}$$

Q: Impeller primary flow [$\text{m}^3 \cdot \text{s}^{-1}$] or pumping capacity.

N: Impeller rotational speed [s^{-1}]

D: Impeller diameter [m]

Impeller Reynolds number

For a Newtonian fluid and mixing tanks, the Reynolds number is given by:

$$Re = \frac{D^2 * \rho * N}{\mu} \quad \text{Equation (5)}$$

where N is the rotational speed of the impeller, ρ is the density, and μ liquid dynamic viscosity [Pa.s].

Experimental methods

Power draw or torque measurement

One of the most vital measurement one make take, is the power draw of the stirred tank mixing system. The power draw P of an impeller described in Equation (2) and Equation (3).

All the mechanical energy from impellers must eventually be degenerate as heat energy. In that case, one way to measure the power draw to measure temperature rise in the fluid over time. In fact, it is very hard to measure to do it precisely, because of effectiveness of the insulation. It is also problem with fluids physical properties, because they are dependent on temperature. That is the reason that those methods are not often used. Methods based on reaction torque of the system are more suitable.

Several other methods are available to measure reaction torque. Some of the methods measure the individual torque for each impeller separately. However, others allow only for the whole torque system. It is not important which methods are used, but important is that the torque device is properly calibrated over the range of torque value being measured, free of error caused by friction, and compensated for any temperature effects. Some of the methods to measure of torque are Strain Gauges, Air bearing with load cell, shaft power measurement using a modified Rhymester etc. [1]

Flow measurement technique

Before numerical methods were developed, the research about turbulence flow fields was based on statistical analysis. Theoretical progresses in the field have been done by experiments that included pressure measurements by points and by method (HWA) Hot wire anemometry. However, HWA technique has been less used in experiments, because of its difficulty, whereas in others, corrections have been introduced to the measurement results. After the invention of the laser in the 1960s, the technique of laser Doppler anemometry (LDA) was developed by scientists. In the last 30 years, the LDA technique has been more developed.

Three-component fiber optic based LDA systems with frequency-domain signal processors are per today the highest development and used in several facilities. The addition of a second photodetector to the first component LDA receiving optics results the system the ability of size measurement, in addition to velocity, through phase difference analysis of the scattered light.

Phase Doppler anemometer

(PDA) is an extension of the LDA and is an important tool for size determination of spherical particles. From early 1960s, the investigation of 3D coherent structures has been of significant interest for turbulence researchers. Flow visualization techniques have been around since the days of Prandtl. Flow markers, such as seeding particles, smoke, and so on, are typically used, and the techniques have been improved, with new ones being developed over the years. The evolution of these whole field flow visualization techniques has led to quantification of the visualized results, especially during the last decades with the advent of digital imaging and fast growth of computational power. Particle image velocimetry (PIV) has evolved to be a highly powerful technique for 2D and 3D whole field velocity measurements, while planar laser-induced fluorescence (PLIF) is also becoming a powerful technique in the mixing research community for quantitative concentration measurements. [1]

Nonintrusive Measurement Techniques

In past an extra attention was in the development of nonintrusive flow measurement techniques and methods for measuring vector as well as scalar quantities in the flow. All techniques are based on optical approaches. A short overview of some of these nonintrusive measurement techniques are mentioned below.

Particle Tracking Velocimetry and Laser Speckle Velocimetry.

Just like PIV, PTV and LSV measure instantaneous flow fields by recording images of suspended seeding particles in flows at successive instants in time. An important difference among the three techniques comes from the typical seeding densities that can be dealt with by each technique. PTV is appropriate with low seeding density experiments, PIV with medium seeding density, and LSV with high seeding density. The issue of flow seeding is discussed later in the chapter. Historically, LSV and PIV techniques have evolved separately from the PTV technique. In LSV and PIV, fluid velocity information at an interrogation region is obtained from many tracer particles, and it is obtained as the most probable statistical value. The results are obtained and presented in a regularly spaced grid.

In PIV, a typical interrogation region may contain images of 10 to 20 particles. In LSV, greater numbers of particles in the interrogation region scatter light, which interferes to form speckles. Correlation of either particle images or speckles can be done using identical techniques and result in the local displacement of the fluid. Hence, LSV and PIV are essentially the same technique, used with different seeding density of particles. In the rest of the chapter the acronym PIV is used to refer to either technique. In PTV, the acquired data provide a time sequence of individual tracer particles in the flow. To be able to track individual particles from frame to frame, the seeding density needs to be small. Unlike PIV, the PTV results in sparse velocity information located in random locations. Guezennec has have developed an automated three dimensional particle tracking velocimetry system that provides time-resolved measurements in a volume. [4]

Image Correlation Velocimetry. This method introduced image correlation velocimetry (ICV) for the purpose of measuring imaged fluid motions without the requirement for discrete particles in the flow [5]. Many other methods were developed. Although such developments are novel, we are still far from being able to fully characterize a flow by

complete simultaneous measurements of density, temperature, pressure, and flow velocity.

LASER DOPPLER ANEMOMETRY

Laser Doppler anemometry is a nonintrusive technique used to measure the velocity of particles suspended in a flow. If these particles are small, in the order of micrometers, they can be assumed to be good flow tracers following the flow with their velocity corresponding to the fluid velocity. The LDA technique has some important characteristics that makes it an ideal tool for dynamic flow measurements and turbulence characterization.

3. COMPUTATIONAL FLUID DYNAMIC

Computational fluid dynamics (CFD) is a tool for solving conservation equations for mass, momentum and energy in flow geometry of interest. Flows and associated phenomena can be described by partial differential equations, which are in many cases extremely difficult to solve analytically due to the non-linear inertial terms. To obtain accurate results the domain in which the partial differential equations are described, has to be discretized using sufficiently small grids. Therefore, accuracy of numerical solution is dependent on the quality of discretization used. [6]

Turbulence modeling

Turbulent modelling is the construction and use of a model to predict the effects of turbulence. Averaging is often used to simplify the solution of the governing equations of turbulence, but models are needed to represent scales of the flow that are not resolved [7].

Table 2. Turbulence models and their description

Turbulence Model	Description, Advantages, and Disadvantages
Standard $k-\epsilon$	The most common used model, it is robust and quite cheap. Has been useful in engineering community for many years. It gives stable calculation and are very suitable especially for high Reynolds number. Not useful for swirling flows.
RNG $k-\epsilon$	One developed model of the $k-\epsilon$, this model improved results for swirling flows and flow separation. However, the disadvantages is that the model is less stable than standard $k-\epsilon$ model.
Realizable $k-\epsilon$	Another adjusted version of the $k-\epsilon$ model, the realizable $k-\epsilon$ model correctly predicts the flow in round jets and is also well suited for swirling flows and flows involving separation.
RSM	Good estimates for all types of flows, including swirl, separation, and round and planar jets. Because equations for the Reynolds stresses are

	solved directly, it is more expensive than $k-\epsilon$ models. The reason is longer calculation time.
LES	Large eddy simulation is a transient formulation and offer good results for all flow systems. The model is based on Navier–Stokes equations and calculate large-scale turbulent fluctuations and models only the small scale fluctuations. Because it is a transient formulation, the required more time for calculation than the RSM and $k-\epsilon$ s. In addition, a finer grid is looked-for to achieve the maximum benefit from the model and to accurately capture the turbulence in the smallest, subgrid scale eddies. Analysis of LES data require a bit higher advance planning and work.
$k-\omega$	This is another two-equation model. In this model ω is an inverse time scale that is associated with the turbulence. Its numerical behavior is similar to that of the $k-\epsilon$ models
DSM	<p>DNS is conceptually the simplest approach to the problem of turbulence. An initial velocity field is assumed and iterated and the velocity field is evolved over time.</p> <p>DNS requires considerable resources. The scale for the resolution of small eddies is at least 1000 times smaller than those used in LES.</p> <p>DNS is the leading edge of turbulence research. So far only basic problems are being addressed. Applications of DNS can be used to study fundamental properties of turbulence, provide data to compare simplified turbulence models, and simulate other effects such as non-Newtonian phenomena.</p>

Numerical methods

Conservation Equations in differential form describe the fluid movement on fluid in time and space. Before one starts to solve those equations numerically, it needs to be discretized or change its form from continuous to discontinuous. For instants, the region or volume the fluid are passing by, it has to be defined by a number of connected volumes, or small cells (mesh). It is necessary for the equations to be written in an algebraic form.

The equations themselves need to be written in an algebraic form. Advancement in time and space needs to be described by small, finite steps than the infinitesimal steps. All of these processes are collectively defined as discretization.

Discretization of the Domain: Grid/mesh Generation

To break the volume or region into a set of discrete pieces, or computational cells, or control volumes, a grid is used. Also called a mesh. The grid can be in many shapes and sizes. In 2D for example the elements are either quadrilaterals or triangles. In 3D have a look at Figure 2. They can be tetrahedral, prisms, pyramids, or hexahedra. The difference between shapes are just number of corner sides. A series of line (2D) or planar faces (3D) connecting the boundaries of the domain are used to make the elements.

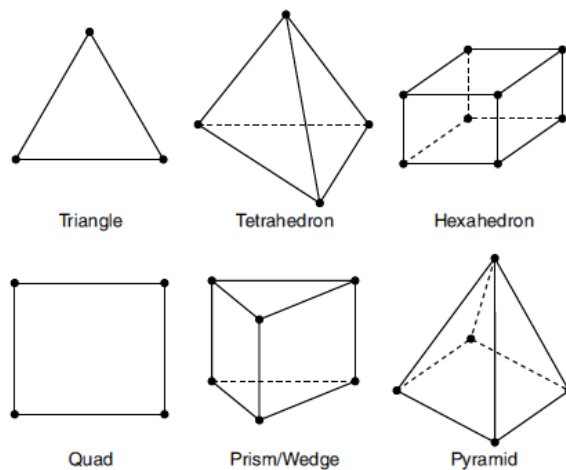


Figure 2. Mesh elements type [1]

Alternative Numerical Techniques

Finite Difference Method

The finite difference/Taylor series formulation replaces the derivatives with finite differences evaluated at the variable storage sites using a truncated Taylor series expansion. The differences for each variable are computed using the cell value and/or the adjacent neighbor values, depending on the order of the derivative. The variation of the variable between storage sites is ignored during the solution process. The method is acceptable to solve for some problems, however it is not preferred for general CFD analysis because the method is limited to simple grids and does not conserve mass on coarse grids.

Finite Element Method

The finite element method uses quadratic functions to describe the variation of the variable within a cell. By connecting the selected function into the conservation equation for each cell and applying the boundary conditions, a linear system of coupled equations is obtained. These equations are then solved (iteratively) for the unknown variable at all storage sites.

This method is popular for use with structural analysis codes and some CFD codes. In the early days of CFD, when structured orthogonal grids were used for most applications of the finite volume method, the finite element method offered the luxury of unstructured meshes with non-orthogonal elements of various shapes. Now that the use of unstructured meshes is common among finite volume solvers, the finite element method has been used primarily for certain focused CFD application areas. In particular, it is popular for flows that are neither compressible nor highly turbulent, and for laminar flows involving Newtonian and non-Newtonian fluids, especially those with elastic properties.

Solution methods

Discretization process results a finite set of coupled algebraic equations, which has to be solved by simulation in every cell in the solution. It requires an iterative solution procedure, because of the nonlinearity of the equations that run the fluid flow and related process. Two methods are often use. A segregated solution approach is one where a variable at a time is solved in the whole domain. Therefore, for the velocity x component is solved for the whole domain, thereafter y component is solved, and it continuous like that. The other solution approach is one where all variables, momentum and continuity are solved simultaneously in a single cell before the solver moves to the next cell, and the process is repeated with the same procedure.

Simple Algorithm

For three dimensions simulations, the three equations of motion and the equation continuity combine to form four equations for four unknowns. Among the unknown components, one is pressure and three velocity. Pressure has no explicit equation that is why some unique techniques has been created to extract it in an alternative manner. The well-known technique is SIMPLE algorithm. The principle of the algorithm is as follows.

An estimated pressure field is used in the solution of the momentum equations. Then starts to compute a new velocity, but these in general will not fit the continuity equation, so corrections to the velocities are determined. Based on the velocity corrections, a pressure correction is computed which when added to the original guessed pressure, results in an updated pressure. Following the solution of the remaining problem variables, the iteration is complete and the entire process is repeated.

Convergence criteria

This criteria are specific condition for the (usually normalized or scaled) residuals that define when an iterative solution is converged. Once converge criterion can be that the total normalized residual for the pressure equation drop is under 10^{-3} . Alternatively, it might be the total scaled residual for a species equation drop is under 10^{-6} . Instead, it could be that the sum of all normalized residuals drop is below 10^{-4} . Whatever set of convergence criteria, the guess is that the solution is stable with no change when the condition gotten and that there is an overall mass balance through the domain. When supplementary scalars are being solved for example heat, there should be overall balances in the scalars too. While the convergence criteria indicated that, overall balances probably exist. [1]

Residuals

The residuals are the error magnitudes for Equations as iterations progress. The equations include the governing equations for example Navier-Stokes momentum equation for each direction (x, y, and z of 3D or just x and y for 2D). The residual is the difference between the previous result and the current result. As these errors are falling, the equation results are reaching values that are changing less for each time. [8]

Simulation of moving parts

Rotating Frame Model

The rotating frame model solves the momentum equations for the entire domain in a rotating frame.. Problems solved in a rotating frame typically use the angular velocity of the primary rotating component, as the angular velocity of the frame. In stirred tanks, the impeller serves this purpose, so the frame is counted to rotate with the impeller. Thus, the impeller is at rest in the rotating frame. The tank, however, rotates in the opposite

direction, so must have a rotational boundary condition. If baffles exist, they would need to rotate into the fluid with the same angular velocity. Unfortunately, this simple steady-state model is not equipped to handle the motion of elements such as baffles into or through the fluid. The approach is therefore only useful for un-baffled tanks with smooth tank walls that are geometrically equivalent to a perfect surface of revolution. Thus an un-baffled cylindrical tank with an axisymmetric bottom shape and no angular-dependent internals could be simulated in this manner. Vessels with baffles, dip tubes, or inflow–outflow ports could not.

Multiple Reference Frames Model

Multiple Reference Frames model MRF are a modified from the Rotating Frame model. In the modification several rotating or nonrotating references frame can be used in calculation. The rotating frame is utilized for the region with rotating components; meanwhile the stationary frame is used for the volumes that are stable or stationary. In the approach rotating frame, the impeller are not moving. In stationary frame with tank walls and baffles, the wall and baffles are not moving. In that case, multiple reference frames can be used as well, that means the multiple impeller shafts in a rectangular tank can be modeled separately with rotating frames. While the remaining space can be modeled with a stationary frame

Sliding Mesh Model

SM approach is a time-dependent solution, where the mesh around the rotating part(s) physically moves during the solution. The velocity of the shaft and impeller compare to the moving mesh region are close to zero. As is the velocity of the tank, baffles and other internals parts in the stationary region.

The motion of the impeller is realistically modeled because the grid surrounding moves as well, and that giving rise to a time-accurate simulation of the impeller–baffle interaction. The motion of the grid is not continuous. It is in small, discrete steps. After each such motion, the set of conservation equations is solved in an iterative process until convergence is reached. The grid moves again, and convergence is once again obtained from an iterative calculation. During each of these quasi-steady calculations, information is passed through the interface from the rotating to the stationary regions and back again.

In order to rotate one mesh relative to another, the boundary between the meshes needs to be a surface of revolution. When in its initial (not rotated) position, the grid on this boundary must have two superimposed surfaces. During the solution, one will remain with the rotating mesh region, and the other will remain with the stationary mesh region. At any time during the rotation, the cells will not (necessarily) line up exactly, or conform to each other. When information is passed between the rotating and stationary grid regions, interpolation is required to match each cell with its many neighbors across the interface.

The sliding mesh model is the most rigorous and informative solution method for stirred tank simulations. Transient simulations using this model can capture low-frequency (well below the blade passing frequency) oscillations in the flow field. [9]

4. SOLUTION PROCEDURE

It is a transient model involving the motion of the impeller, starting the simulation with the impeller at rest is analogous to modeling startup conditions. After a while of time the flow field gets periodic steady state, but this period of time may correspond plenty of revolutions. If the goal of the simulation is to study the periodic steady-state conditions, decreasing the time spent reaching this state is necessary.

The way to go through the startup conditions is to move the impeller by large increments each time step in the early stage of the calculation. If the model is a 90° sector, for example, the first few revolutions of the impeller can be modeled using a coarse time step that corresponds to a 30° displacement. The time step can then be refined to correspond to a 10° displacement, and refined again (and again) until the desired temporal and spatial accuracy is achieved. The solutions during these initial coarse time steps do not need to be converged perfectly, provided that the simulation involves a single fluid phase and there are no inflow and outflow boundaries. In these instances, improved convergence can be obtained in the later stages of the calculation.

An alternative way to bypass calculation of the startup period is to solve for a steady-state solution first using the MRF model provides a solution for the moving impeller at a fixed orientation relative to the baffles. Tools are available in commercial codes to use the solution data from the MRF simulation and apply it to the sliding mesh simulation as an initial condition. A moderately coarse time step can be used initially (say, corresponding to a 10 rotation, as in the example above) and reduced at a quicker rate than would otherwise be advisable. This approach can also be used if inflow and outflow boundaries are present or if a multiphase calculation is to be performed. In the case of multiphase flows, however, care must be taken to wait until the periodic steady-state condition has been reached before introducing the secondary phase.

Summary

After literature research I found out the possibilities to obtain mixer characteristics by direct measurement and experiments such like PIV, PTV, LSV, for velocity profile. To obtain power, we have to measure for each blade separately or together if there were more blades. As the experiments are time consume, therefore some software programs were devolved to simulate the agitate mixer. Among the software that can be used to predict

mixer characteristics is ANSYS FLUENT 2015. ANSYS Fluent software contains the broad physical modeling capabilities. This software are powerful and gives different ways to simulate turbulence flows.

I will use LES and sliding mesh method, because it is the recommended for the stirred vessels. Firstly, I will create geometry and structured mesh and MRF method will be used for initial prediction of velocity and pressure field. Thereafter, the model will be switched to transient mode and LES approach will be setup. Then the simulation will let be stabilized for certain time. After that with respect to required revolution, the model will be simulated for e.g. 10 seconds. Required data will be recorded. In post processing these data will be performed as averaged values.

SIMULATION

Pre processing

One can check the flow regime by using Equation 5 for the agitate vessel with a speed 300 m.s^{-1} . The Reynolds number for the impeller Re was 500000. By all confidence, this regime is fully turbulence: $500000 > 3200$. The mixed liquid is simplified in this work to be pure water. The geometry below were chosen with respect to well-known experimental data. In this report LES approach will be used, because MRF method was not able to give good simulation results. [10]

Geometry creation

There are several Software programs available to create geometry. Among them Pro Engineering, Solids Works etc. One might create the geometry from one of the mentioned programs and transfer it to Ansys workbench for further work. Firstly, we created geometry of a single impeller within a vessel, including four baffles on sides. This geometry was created in Solids works. After transferring to Ansys and performed an operation so called boolean operation to create initial volume of fluid and remove the solid bodies in this case impellers, shaft and baffles, look at Figure 3 below:

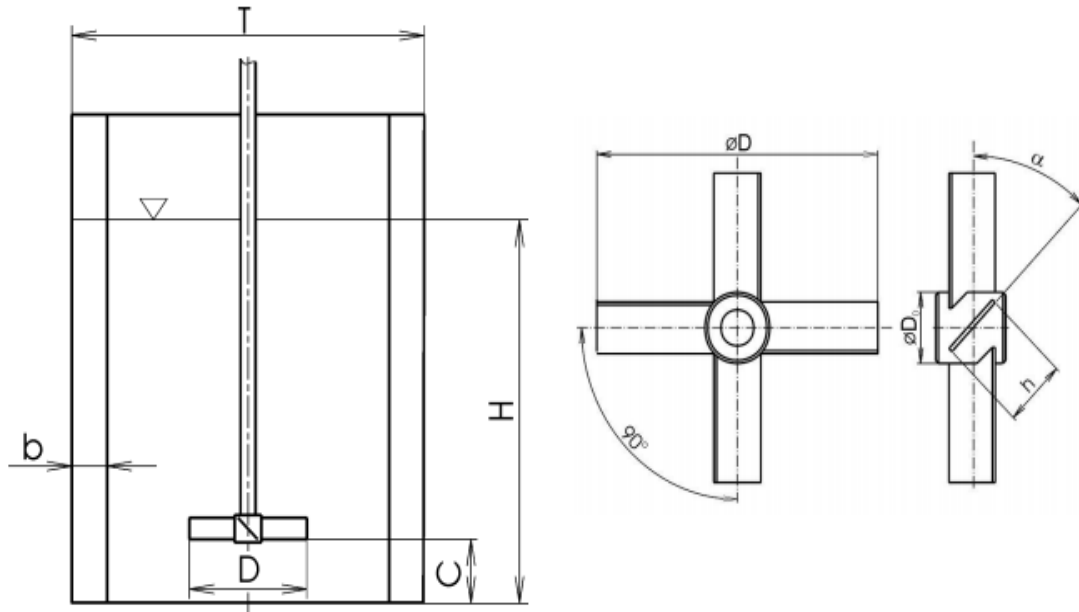


Figure 3. Sketch of the stirred tank and impeller. [10]

Table 3. Dimensions of the vessel and impeller

Dimension	Length, size
T	300 mm
H/T	1
D	100 mm
C/D	1
b/T	1/10
Bi (number of blades)	4
α	45°
h/D	1/5
n	300 per min

Next step after geometry creation is meshing. However, before start with the mesh process, the volume has to be sliced into smaller volumes. One cylindrical volume around impeller with a distance two mm far from the impellers. Those surfaces were created due to easy way to evaluate flow rate from the impeller and their flow rate number. In addition, another bigger cylindrical volume around the impeller for the MRF solution. The MRF volume has distance 50 cm distance from top and button of the impeller. Moreover, 50 cm from sides. The rest of the volume where divided into smaller volumes. The purpose

with volume division is to make it easier for mesh-creation. With smaller volumes, we can choose specific mesh density for specific places.

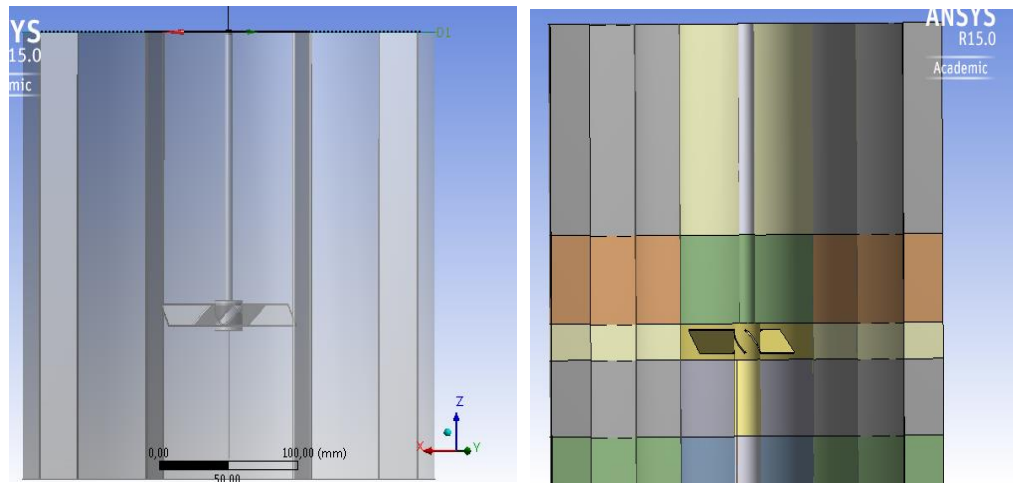


Figure 4. Model of mixing vessel (on the left), Sliding of the model (on the right).

Meshing

After finishing the geometry creation, and separation of the volumes, and make it easier to define boundary conditions the mesh was created. The operation can be also useful to define the motion of the system and analyses of simulation in fluent. After Geometry were ready, we started with mesh. Mesh generation is one of the most critical aspects of engineering simulation. Too many cells might result in long solver calculation. With too few mesh elements are risk for not having exact results compare to experimental results. However, after some mesh techniques and operation, we start with approximately 75437 elements. The region close to the impellers was relative complex geometry that is why tetrahedral mesh type was introduced. Moreover, hexahedron type for the rest of the volumes. During the mesh processing, the sweep method were applied for sweep-able volumes.

Fluent

After creating of mesh, one has to put right set-up in fluent with desirable values. As it is mentioned in theory, there are several alternative methods we can choose to make a turbulence model. LES method are investigated. The fluent has to be modified once for the MRF method and once for the LES method. LES stands for Large Eddy Simulation

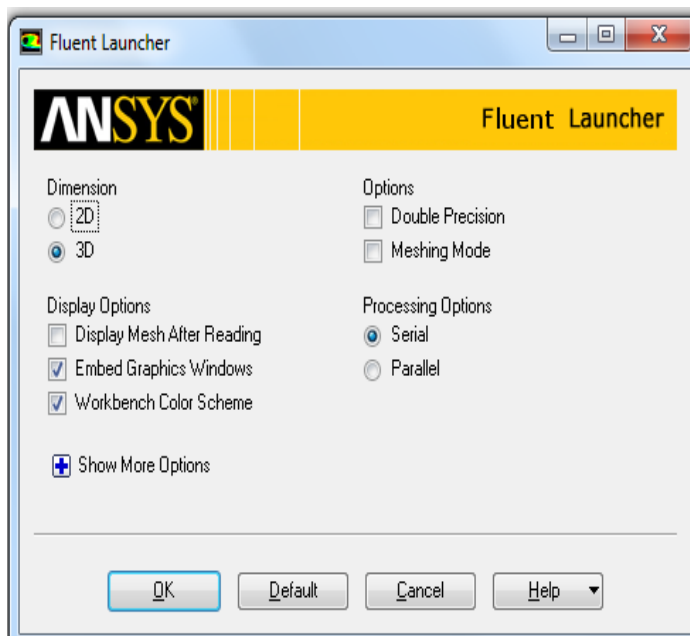
gives solution, which depends one time. That is the reason to apply firstly MRF method to obtain initial values for the LES method. Detail set up are showed below

Setting Up the CFD Simulation in ANSYS FLUENT

Now that we have mesh model for the agitate mixer geometry, in this section we are going to describe detail setups for Ansys fluent with parameters. These process steps of simulation setup will serve as methodology and manual for simulation of stirred vessel by LES method for students of Department of Process Engineering.

FLUENT Launcher

We have to make sure that proper option are selected. Annotation that the



dimension setting is set up automatically and cannot be changed direct. If our geometry were or mesh were 2D, it will choice 2D by its self. The ANSYS FLUENT settings file “FFF.set”. are written once ANSYS FLUENT opens.

Figure 5-Fluent Launcher setup

General

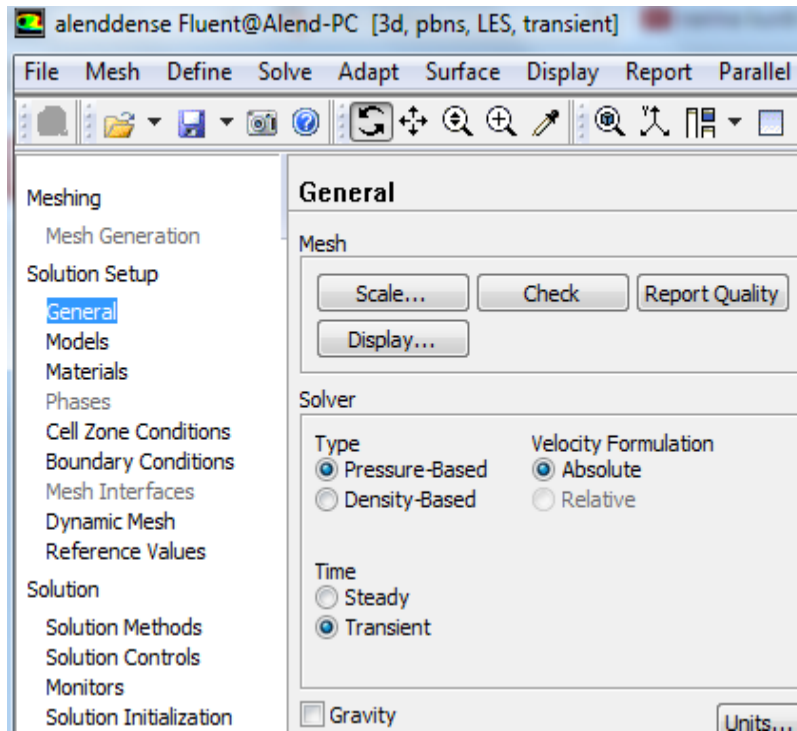


Figure 6-Solution setup-general

General Settings gives solver options of pressure, velocity and Time. As for time if the solution is LES method, Transient has to be selected. Otherwise, Steady has to be selected when we simulate with the MRF approach. Here is also possible to check the mesh quality and get the report. Here we changed unit in Display.

Models

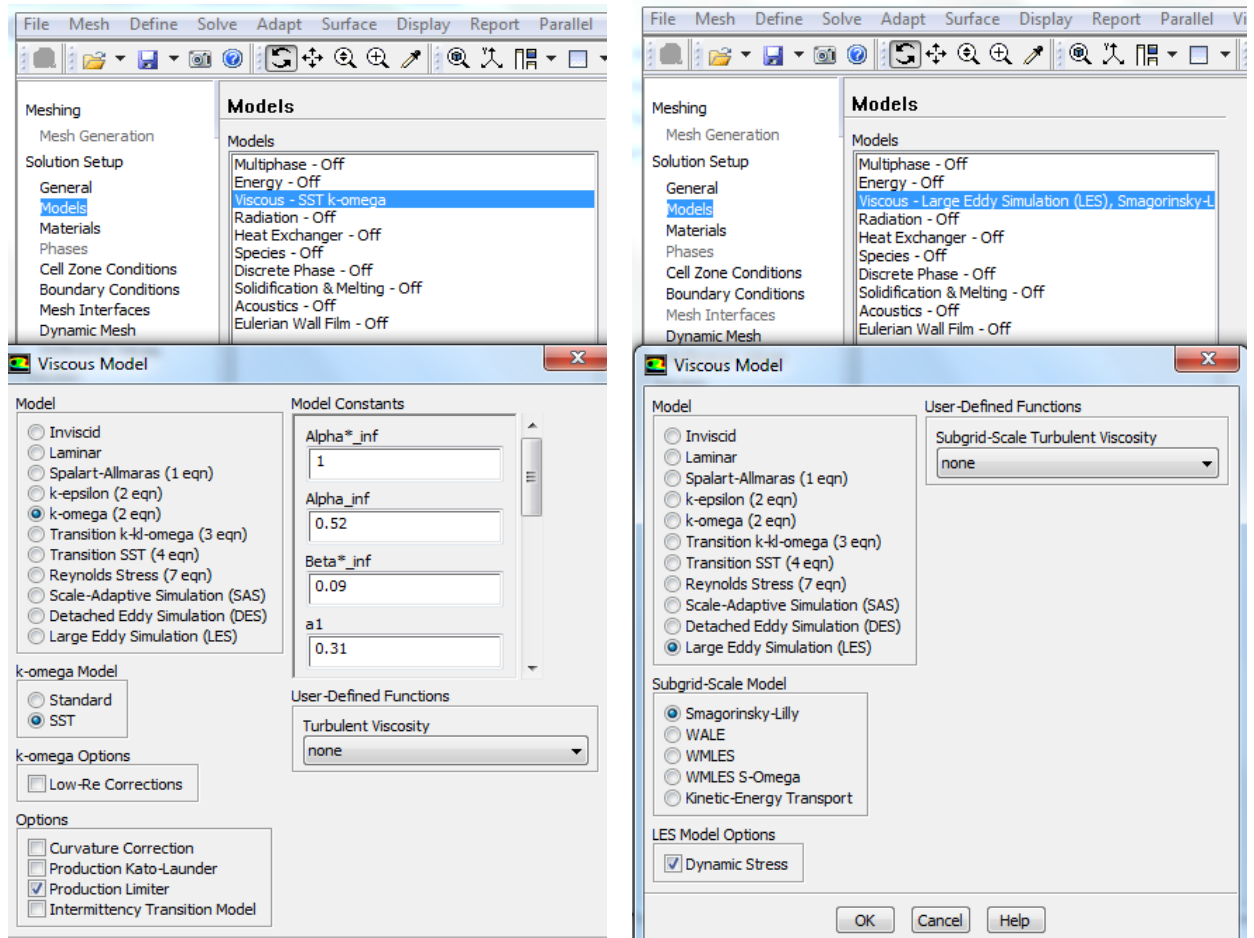


Figure 7. General model setup for k-omega MRF (left side) General model setup for LES (right side)

The subgrid-scale stresses ensuing from the filtering operation are unknown, and require modeling. The subgrid-scale turbulence models in Fluent employ the Boussinesq hypothesis. As in the RANS models, computing subgrid-scale turbulent stresses. As it shows for LES selected Smagorinsky-Lilly and for k-omega SST.

Materials

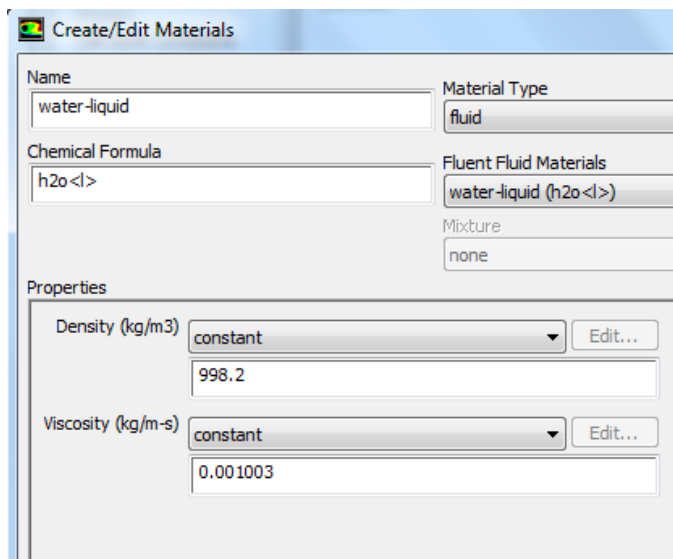


Figure 8. Material setup

For simplification in the project, water was chosen as fluid material in the agitate mixer. After we decide settings for the water properties. Where density was $1000 \text{ kg} \cdot \text{m}^{-3}$ and viscosity $0,001003 \text{ kg} \cdot \text{m}^{-1} \text{s}^{-1}$. It is also possible to change other properties like C_p and thermal conductivity for the given liquid/water condition.

Cell zone and Boundary condition

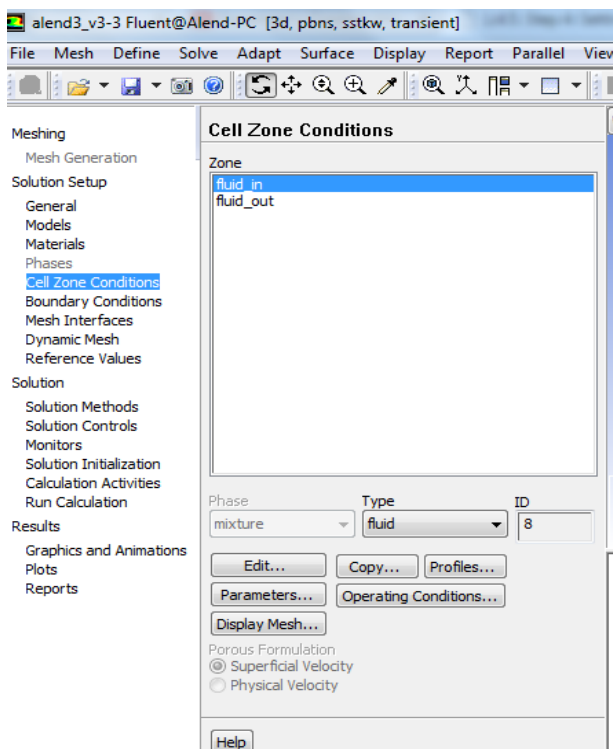


Figure 9. Cell Zone condition setup

“Fluid in” corresponds to the rotating box around the impeller, while fluid out are the outer volume of the box in the vessel. For LES we have to choice mesh motion, while for MRF has to be Frame Motion

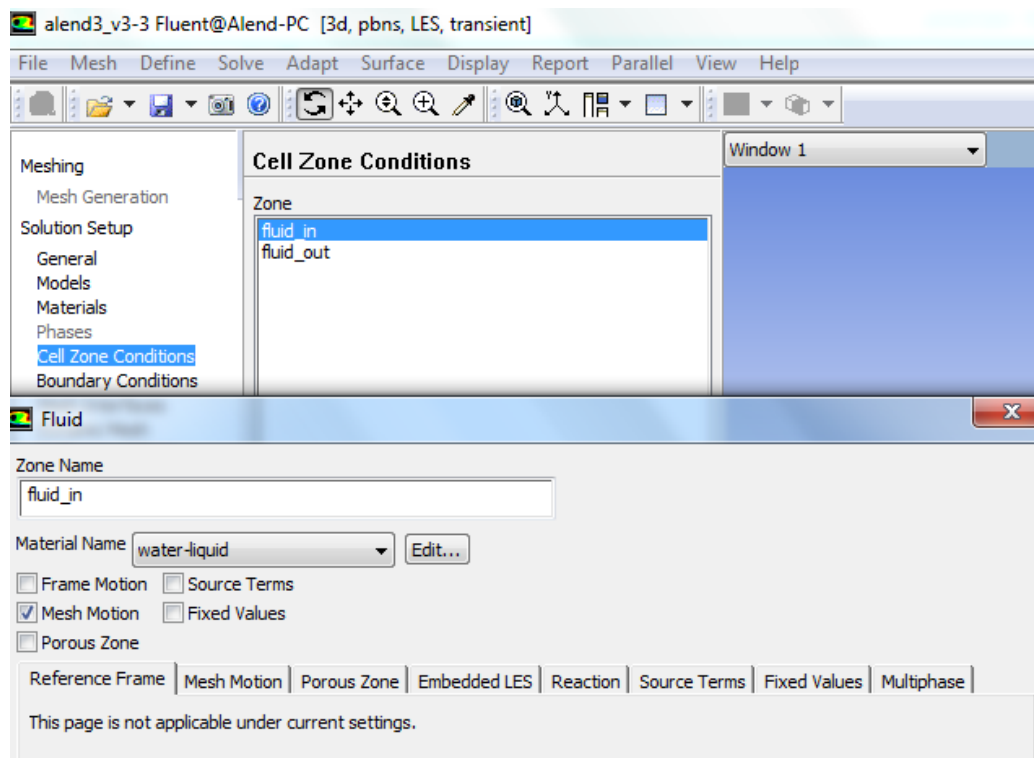


Figure 10. Cell zone condition. (Fluid in setup).

Boundary condition

Below are the table for Name selection and their Boundary condition for the two approaches. As it shows everything are the identically the same, except boundary condition for MRF volume which are interface for LES method and INTERIOR for MRF solution.

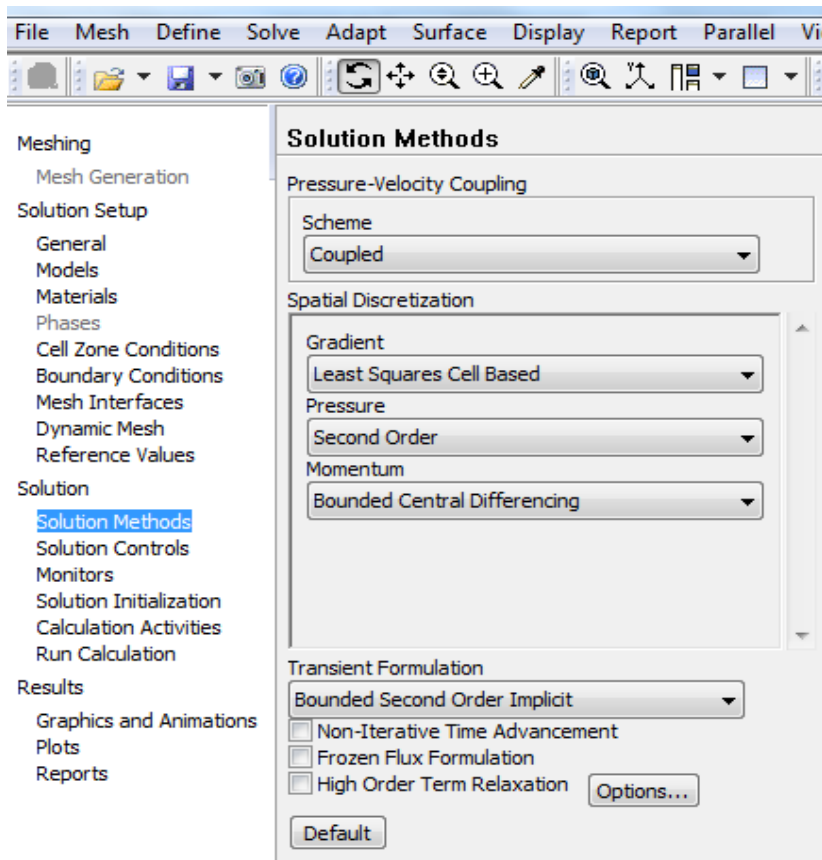
Table 4. Boundary conditions

Name	Surface	Boundary Condition for MRF	Boundary condition for LES
“blades”	All surface of impeller	WALL	WALL
“dshaft”	Down power of shaft	WALL	WALL
“surfup”	Up face of impellers box	INTERIOR	WALL
“surfdown”	Down face of impellers box	INTERIOR	INTERIOR
“surfaround”	Side face of impellers box	INTERIOR	INTERIOR
“baffles”	All baffles	WALL	WALL
“wall”	All outer vessel walls	WALL	WALL
“level”	Top surface of fluid	SYMETRY	SYMETRY
“upshaft”	Upper part of shaft	WALL	WALL
“fluidout”	Surface of the impellers box	INTERIOR	INTERIOR
“fluidin”	Surface of the tank all around the tank	INTERIOR	INTERIOR
“mrf_up”	Upper surface of the the mrf volum	INTERIOR	INTERFACE
“mrf_down”	Down face of the mrf volum	INTERIOR	INTERFACE
“mrf_perp”	Mrf surface on perpendicular side	INTERIOR	INTERFACE

Table 1. Boundary conditions

Solution

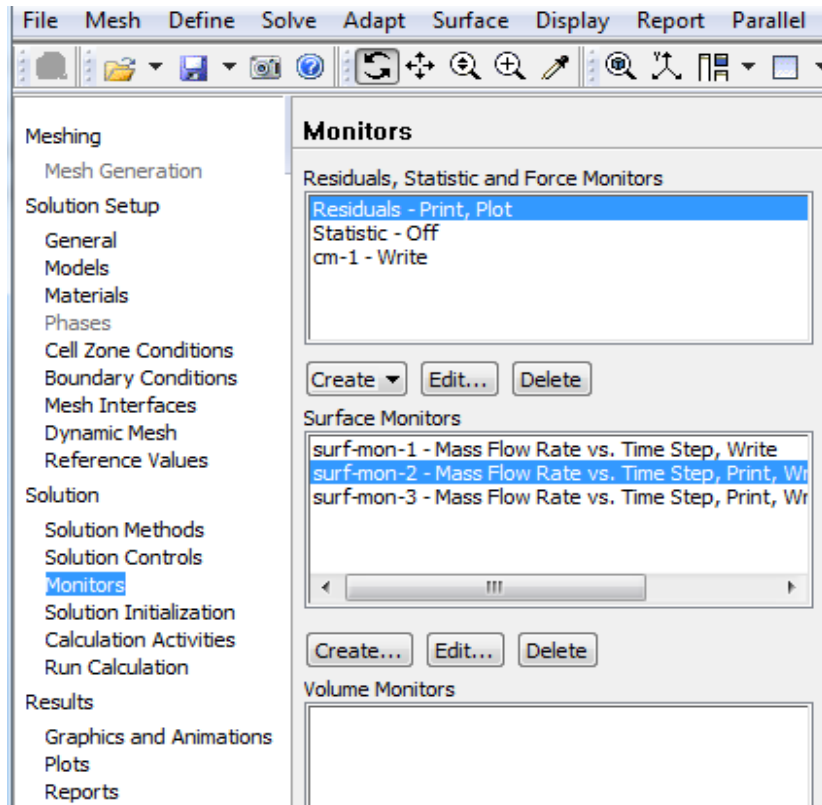
Solution method



It is recommended to choice “Bounded Central Differencing” for momentum solution. And for Transient Formulation “Bounded Second Order Implicit”.

Figure 11.Solution method setup

Monitors



Surface Monitors gives option to obtain reports for different parameters. Here we obtained mass flow rate vs. time step report for those three surfaces around the impeller.

Figure 12. Monitors set

Residual monitors

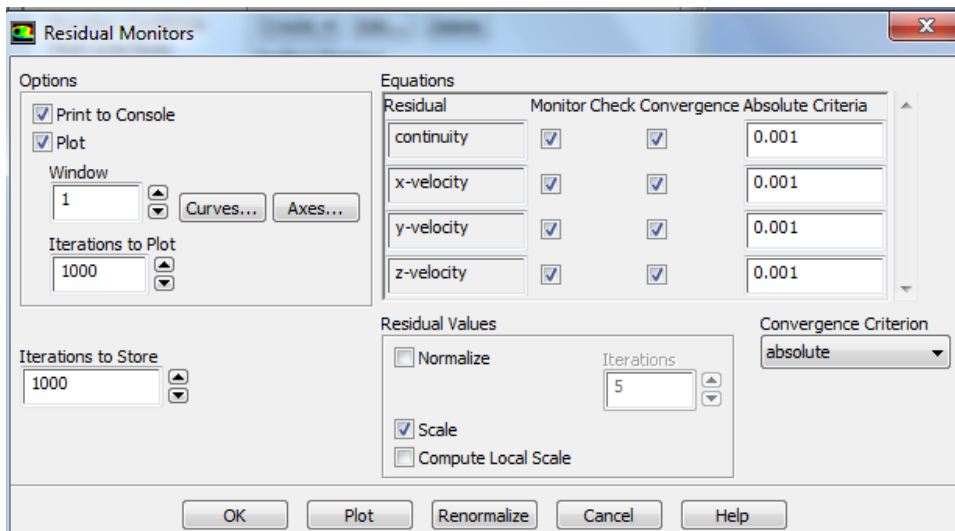


Figure 13. Residual monitors

Solution initialization

Before we start our calculations or patch initial values for selected variables in selected cells we must initialize the flow field in the entire domain. We can also calculate the values from information in a specified zone, enter them manually, or let the program compute average values based on all zones. We can also point out whether the specified values for velocities are absolute or relative to the velocity in each cell zone. In the report, I used Standard Initialization.

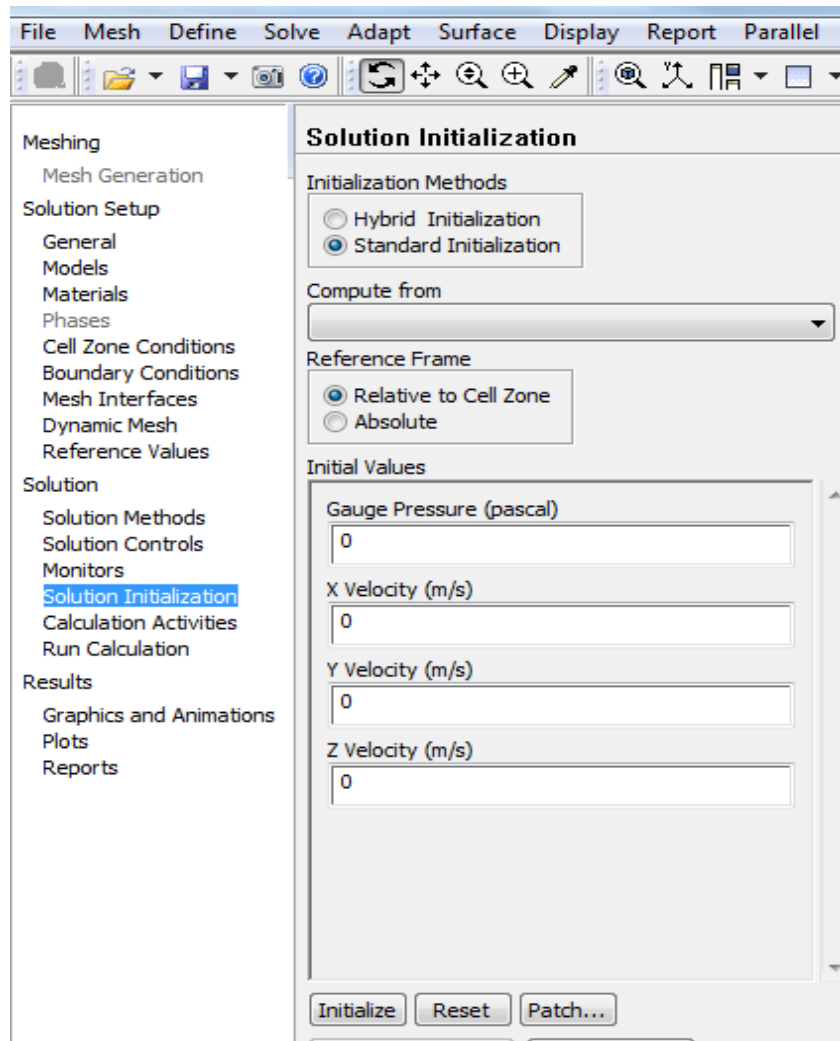
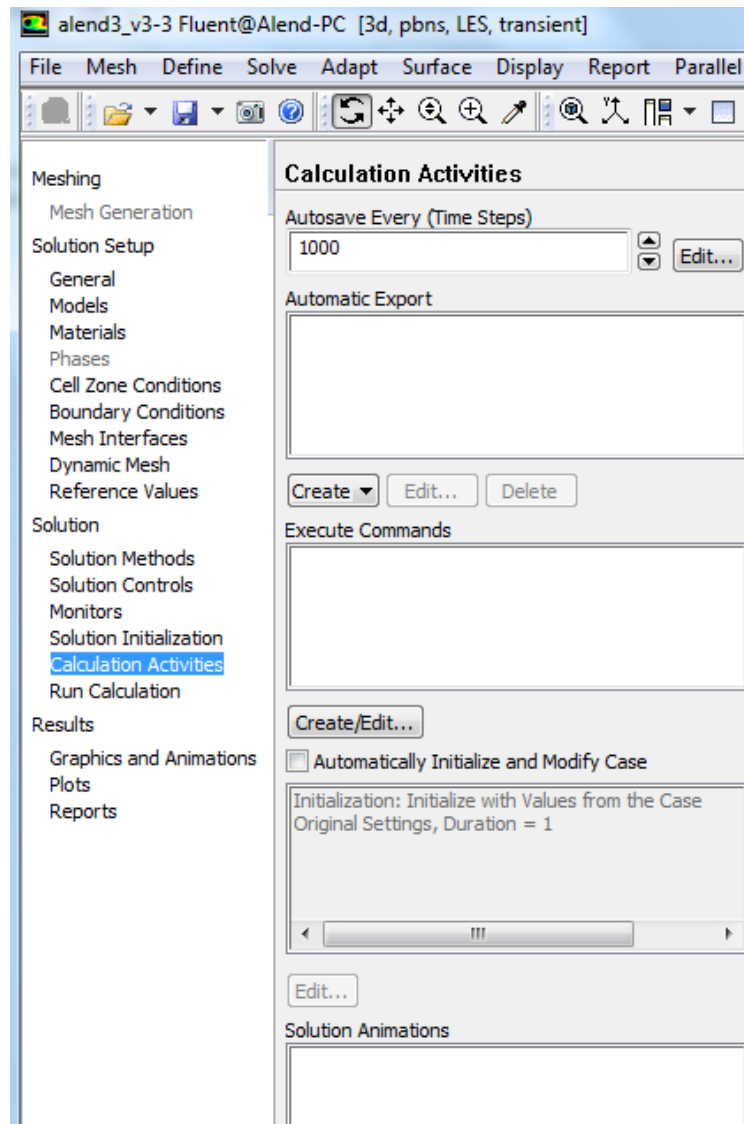


Figure 14. Solution initialization LES setup

Calculation activities

Calculation activities is very useful for long running calculations. For complicated and



significant number of mesh elements, the calculation might takes several days or weeks on computer. The value input for auto save every (time step) saves the calculated values automatically after each given value for AutoSaves Every (time steps).

Figure 15. Calculation activation setup

Run calculation

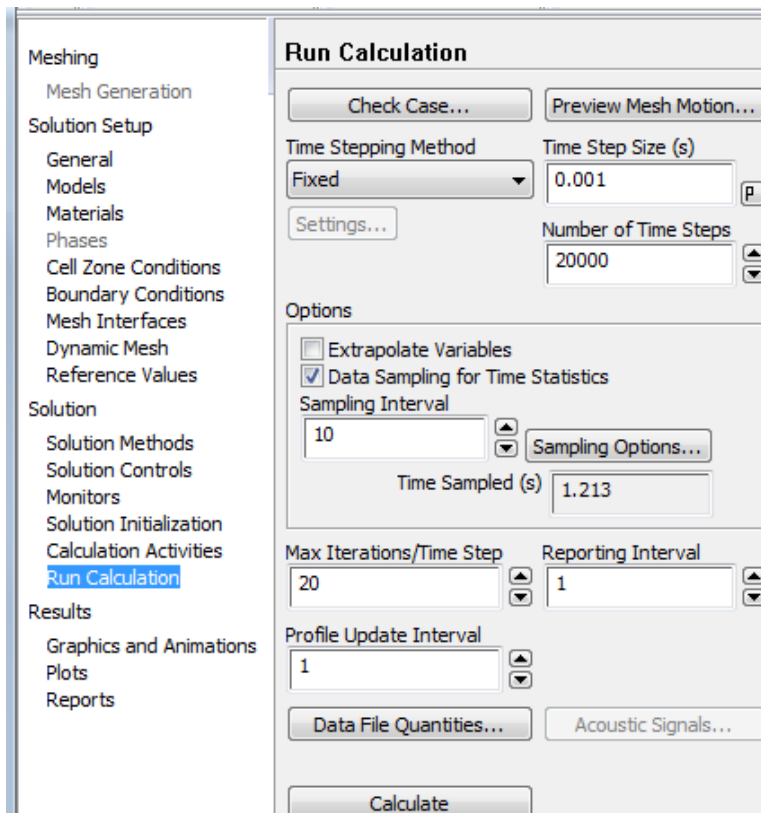


Figure 16. Run calculation setup

For the run calculation we set the time step size (s) to 0.001 s for LES method, and 0.01 s for MRF. This value has to be matched with the rotating speed, when the impellers box are rotating, it should not skip any mesh element. In other words, the step size has to be smaller than mesh element, so all elements will be taken account in calculation. Otherwise it will be less precision in the calculation.

More time step size and more iteration value increase, more time will be necessary for calculation. With those values, it took approximately 48 hours to reach convergence. Check the convergence impulse in the Figure 17.

Residuals

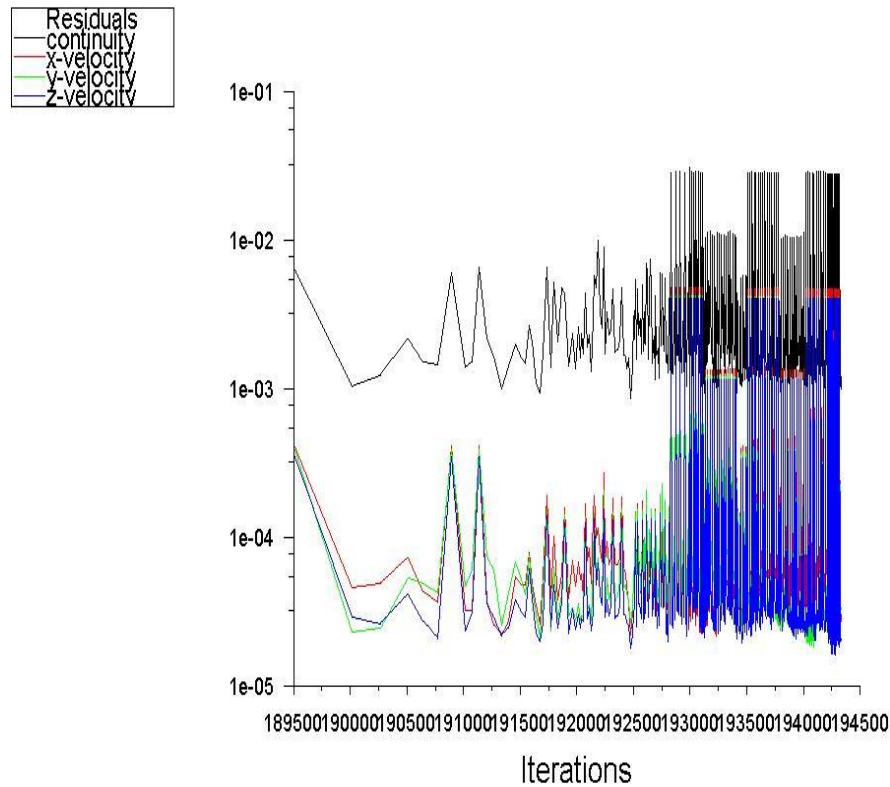


Figure 17. Residual graph

How to check if the convergence have been reached?

- If residuals have decreased to an acceptable degree.

The solution has converged when the Convergence Criterion if each variable has been reached. The default criterion is that each residual will be reduced to a value of less than 10^{-3} .

- The solution no longer changes with more iterations.

Sometimes the residuals may not fall below the convergence criterion set in the case setup. However, monitoring the representative flow variables through iterations could show that the residuals have stagnated and do not change with further iterations.

- The overall mass, momentum, energy, are achieved.

5. FLUENT RESULT

Flow number and flow rate

The flow rate through the rotating impellers was obtained by integrating the velocity field on the surface generated around the impeller. The graph below are the results from simulation. We obtained flowrates for “up”, “down” and “perpendicular” which corresponds to all sides of the box around impeller with respect to time. According to the mass balance, total flow rate for up and perpendicular has to be the same as flow rate for down. In other words we need only the flowrate for “down” to determine flowrate and flowrate number. As the graph shows non-steady state for the flowrate in time. Because of the nature of turbulence, that the follow is not stable. For that reason we calculate the average of mass flowrate and got 4.0325 kg/s. Thereafter we can use the obtained value into the Equation (4) to get flow number or pumping capacity. In the equation, mass flowrate has to be converted to volume flowrate. That means divide the formula by the density of the water $1000 \text{ kg} \cdot \text{m}^{-3}$. Have look at the Table 6 for the flow number result.

$$N_Q = \frac{4,032}{1000 * 5 * 0,1^3} = 0.76 \quad \text{Equation (4)}$$

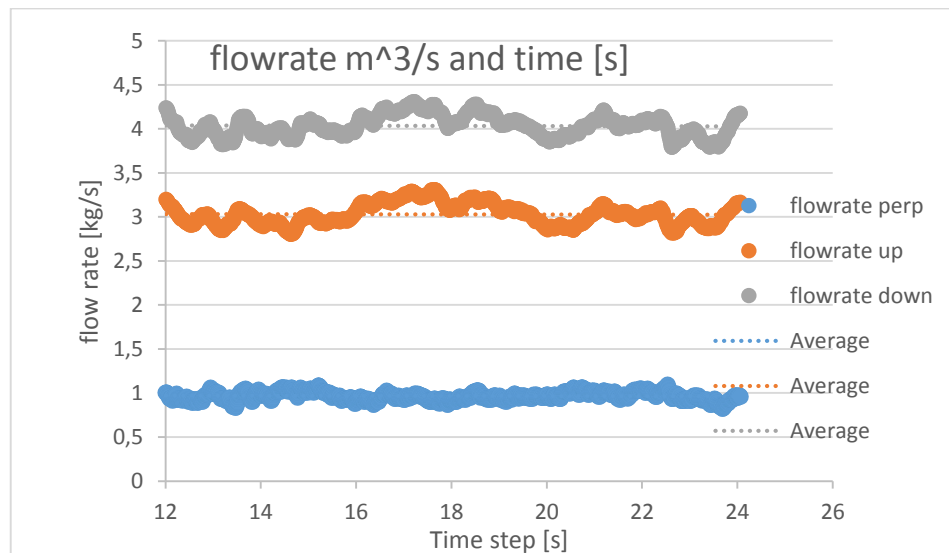


Figure 18. Flow rate passing through the three surfaces around the impeller

First the fluent was setup for MRF approach, which calculate turbulence flow movement. The calculation took 2 days on computer. Thereafter, the calculation was used for LES method as initial value for 12 seconds in real time, which are 5 days calculation on computer. Total real time was in 24 seconds, which means next 5 days. Last 12 seconds were used for post processing. The Figure 18 corresponds to the flow rate in the time range 12-24 seconds for 24000 number of time steps for LES approach.

Creating line for the velocity profile

In the fluent one line below the impeller was scatched. The line Hv is 130 mm long from the shaft surface to the baffles. In addition, 98 mm from down of the tank. It is important that the line has to be in the same latitude as measurement data. Vv line is the vertical line to anaylsis vertical velocity profile and has distanse 2 mm from the impeller. Check the Figure 19. Anaylsing the velocity fluxes on this line and thereafter compare the result with the experimental. Figure 23 are horizontal scheme for experimental apparatus. [11]

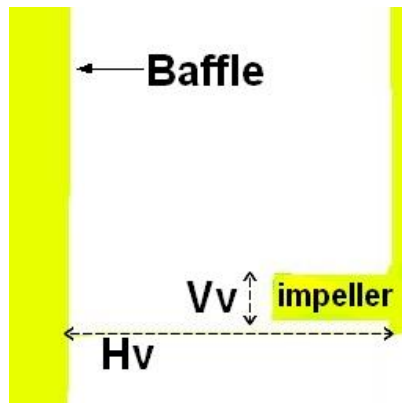


Figure 19. Vertical and horizontal line-creation around the impeller

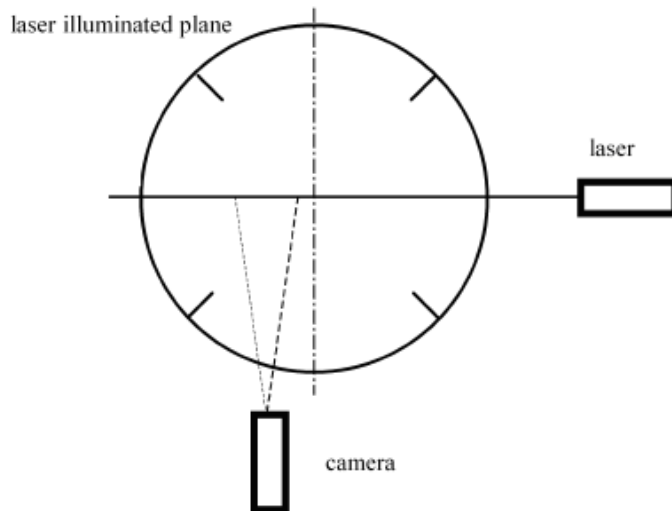


Figure 20. Scheme of the experimental apparatus and the investigated area

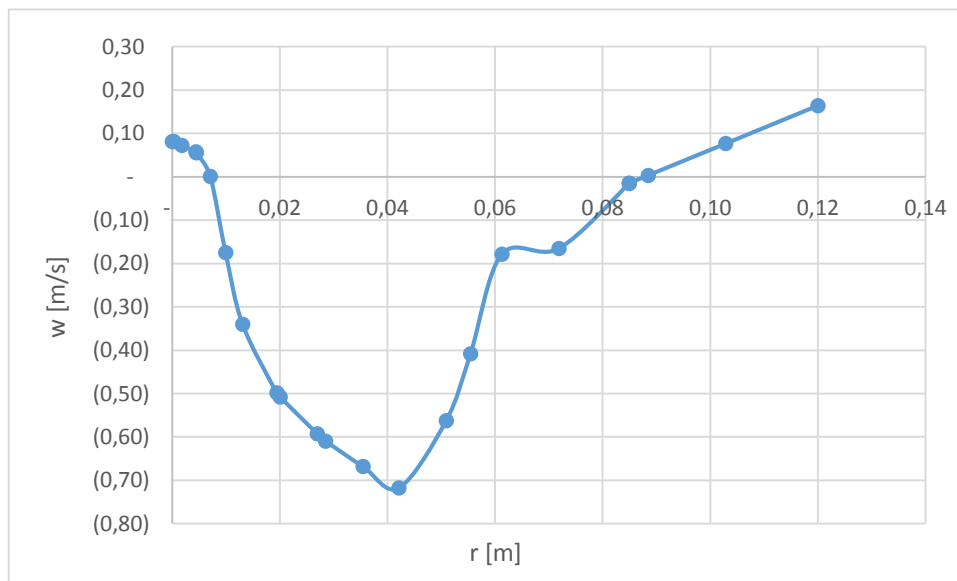


Figure 21. Horizontal velocity profile under impeller (Hv), time averaged, less dense model

Figure 21 explains how are the average velocity developed alongside the created Hv line. It is obvious that the flow under the impeller flows down while the in longer distance

from the impeller water flows up. According to the graph the highest velocity are in the end of the impeller in the point ($W_{max}=-0.72$ m/s, $r_{max}=0,042$ m).

The ensemble-average mean velocity profiles which are function of dimensionless radius R^* and dimensionless velocity W_z^* were investigated in region below the impeller. The dimensionless velocity and radius are calculated as:

Dimensionless velocity:

$$W_z^* = \frac{\overline{W_z}}{\pi \cdot D \cdot N} \quad \text{Equation (6)}$$

Dimensionless radius:

$$R^* = \frac{r}{R} \quad \text{Equation (7)}$$

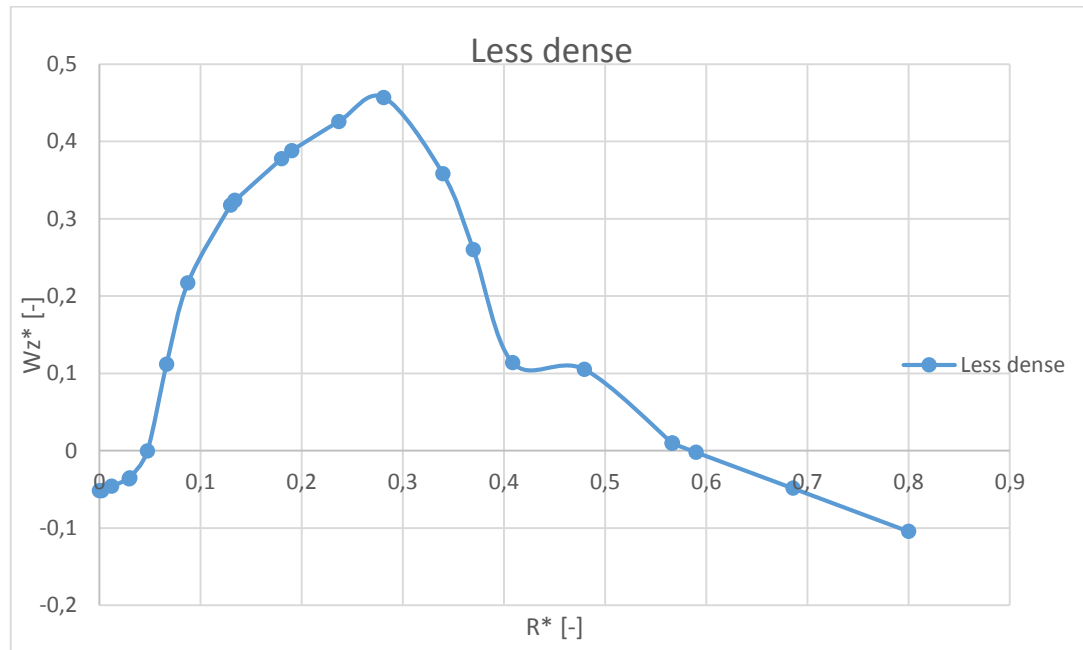


Figure 22. Dimensionless horizontal velocity profile under impeller (Hv) time averaged

Power and torque determination

Power number are one of the main subjective, which has to be found, it is done by several ways. The first way is to calculate Reynolds number for the blades and compare with power number in the Figure 2. The second way is to find the power from the Equation (2) and substitute in the Equation (3) to find power number. The second way are applied. Power is a function of torque; it means torque has to be determined from the simulation. In the fluent software using in-build function, which calculates the torque from the shear stress acting on the user, selected surface. The torque acting on the shaft was neglected, because to a small value. The principle of torque measurement numerically are mentioned and described by the Equation (1).

Table 5. Parameters calculation of less dense model.

Torque Γ [Nm]	0.00125
Power P [W]	1.58
P_0 [-]	1,145
Q [kg*s ⁻¹]	4.0325

Mesh optimization

One of the objective of this task is mesh optimization. As for agitated mixer, the most interest region are the region around the impellers. Because in this region we have to predict power number, velocity profile and other characteristics. From meshing perspective, this region has to be denser than for example top or bottom of the tank. Because the other parts of the tank has not so significant effect on the result. For this purpose, we create another mesh. This time the mesh are not 75437 elements but 459076 elements. It is obvious, more elements require more calculation time. Although the less dense model gave acceptable results, but one can run calculation for the new mesh for more precise result. Below are the picture and tables for the new mesh model.

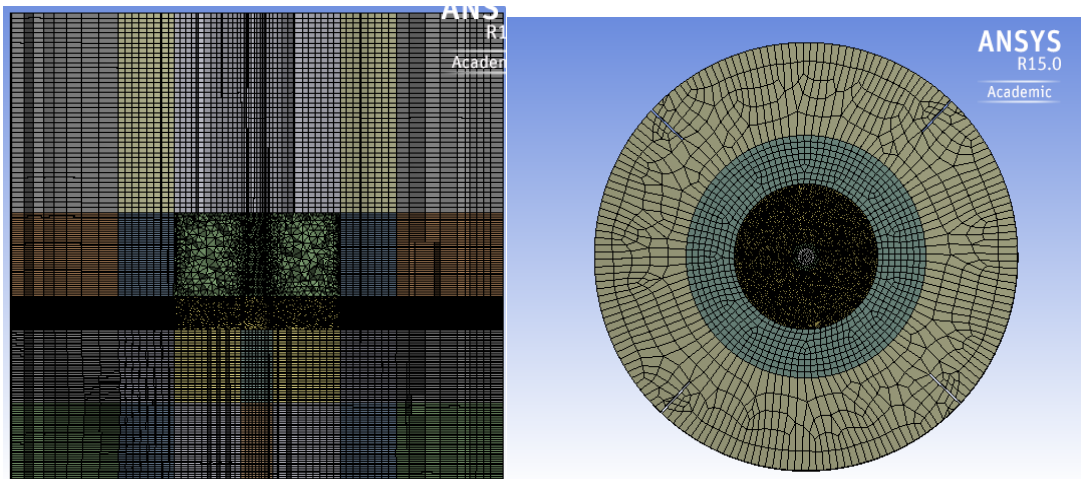


Figure 23. Mesh optimization view, a) right, b) left.

- a) The picture is vertical cross-section of the meshed model. As it shown, it is denser around the impeller than top and down. b) The horizontal cross-section of the model, as it shown close to the cylinders wall has smaller mesh elements and less mesh dense. In reverse to the central has smaller mesh size with denser mesh. Otherwise, the mesh elements types are the same as for first mesh “less dense”, where the tetrahedral are applied for the complex region close to the impellers and hexahedral are applied for the other parts of the tank. For more info about the mesh types, have a look on theory part.
- b) If the mesh quality are poor, it might effects badly on convergense and diffuse solution. There are many technique available on fluent to analysis the mesh quality. One has to make sure mesh quality criteria are within correct range. Check the Figure 28 for acceptable ranges.

Skew factor

One alternative to analysis the mesh quality is that so called skew factor. Skewness is a mersure of the degree of disorder in the distrubution sorrounding a mean value. The skew factor determine the quality of celles to each other. If the neighbouring cells surrounding a single mesh cell are faultlessly symmetrical, thn the skew number are 0. Othersie oppsite, if the neighbouring cells are asymmetrical, the skew number will be higher than 0. The max skew number is 1 for very bed quality of mesh.

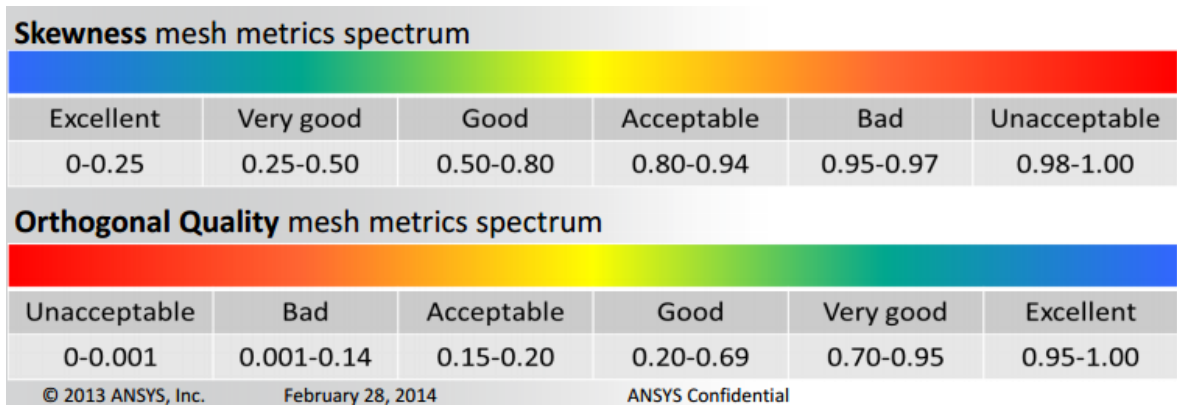


Figure 24. Skewness and orthogonal quality spectrum

Ansys mesh gives many options for mesh quality checking. there were speciall interese to analyse skewness and orthogonal quality. Fiannely, we were able to obtain bar chart for skewnews and orthogonal quality. The bar chart gives spesific number of mesh element types and their quality. As it shows the majority of the elements for skewness are close to the value :0 . According to the metrics specterum, the mesh is in the accebttable region. The same for orthogonal quality, where the the biggest amount of mesh elements are close to the value :1. In genereal we could say the mesh was acceptable, although very small precent of the total mesh element are in unaccepted range. But it will not have a signifiact impct on the result.

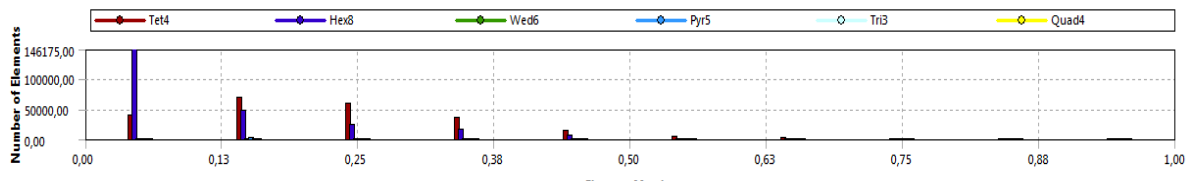


Figure 25. Skewness bar chart for more dense model

Skewness bar chart

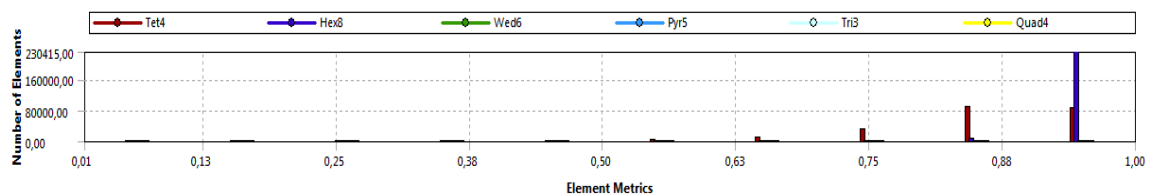


Figure 26. Orthogonal quality bar chart for more dense mode.

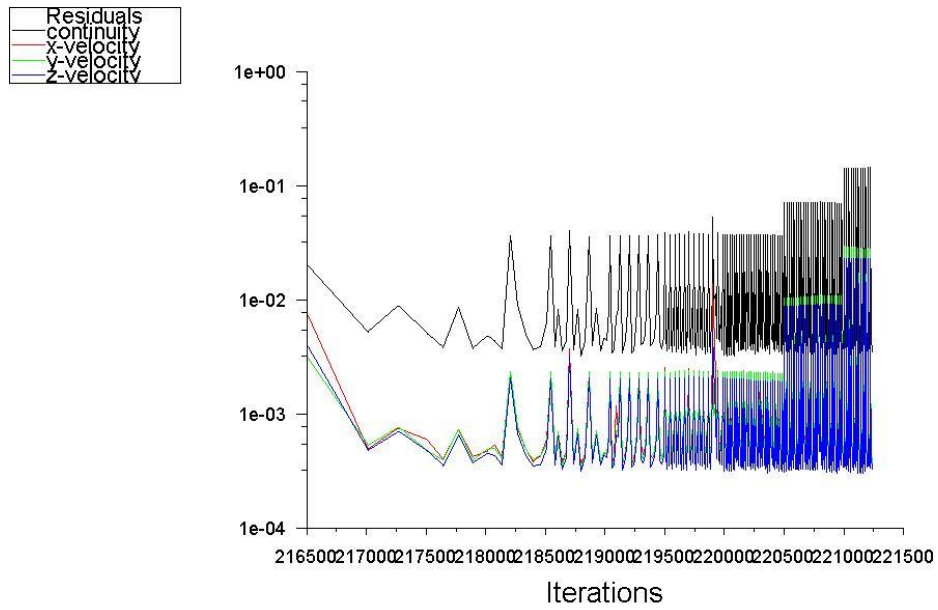


Figure 27. Residuals graph for more dense model

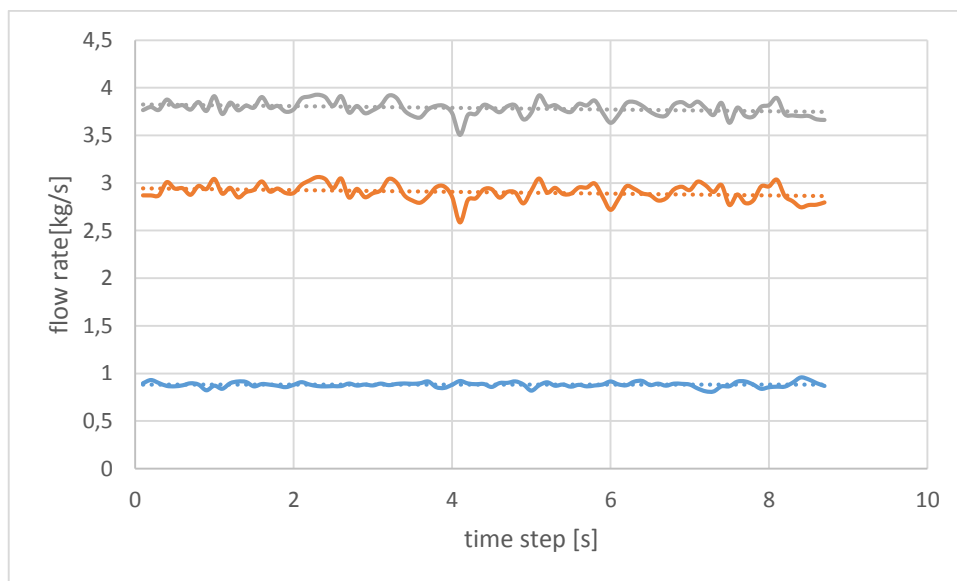


Figure 28. Flow rate passing through the three surfaces around the impeller for more dense model

Discussion and comparison between experimental and simulation model

Table 6 shows the compared result between experimental data of power number, flow number and Ansys fluent simulation. The power number and flow number has been commonly used to check validation of CFD prediction of the flow in the stirred tanks. The accuracy of the power number with the experimental values are -10,7% for the model with “less dense” amount of mesh elements. As for flow number -10,6% accuracy. Simultaneously, the model with high “more dense” presents less accuracy.

Table 6. Experimental data compared with CFD fluent results

	$N_{Qp,exp}$	$N_{Qp,comp}$	$P_{0,exp}$	P_0
less dense	0.85	0.76	1.28	1.145
% accuracy		-10.6%		-10.7%
more dense	0.85	0.71	1.28	1.090
% accuracy		-16.5%		-14.8%

That is the reverse the principle of CFD, where more mesh elements supposed to gives results that is more precise. This error could because of running of calculations with not suitable set-up. The time step for less dens model were 0,001s, while it was reduced to 0,01s for more dense model. The reason for time step decreasing was to decrease calculation time. For the same setup as less dense mesh model, the calculation will takes more than two months. For this reason, time constrains the solution was stopped before it reached the convergence, but as later as possible before finishing this thesis. Have a look at Figure 27. It shows the graph did not fall down enough to reach the stable condition. Ansys fluent required long time to calculation to the less dense mesh model, because of short time, the calculation were stopped before it reached enough in stable condition. That is why in this report only results of less mesh model are represented.

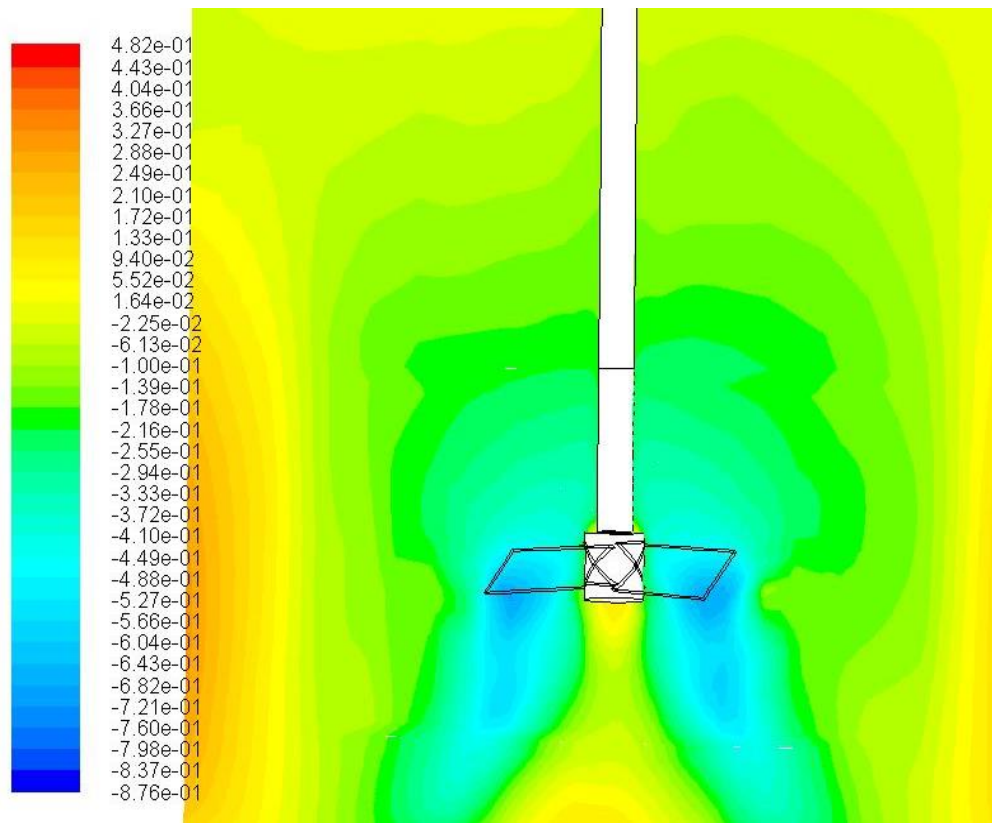


Figure 29. Vertical cut in the plane of the impeller. Contours of mean velocity magnitude. (Less dense model)

Flow field

The model figure 29 was able to predict typical flow field in a for blades stirred tank. The model also shows symmetry from right and left sides, which is one more sign for well-simulated model.

Figure 30 shows the pressure distribution in a cut in horizontal plane through the impeller, showing the region of high pressure in the front and low pressure behind each blade. With the prediction of pressure difference between front and behind sides of the impeller blade and by using Equation (1)-(3), the power number was obtained and compared with experimental data.

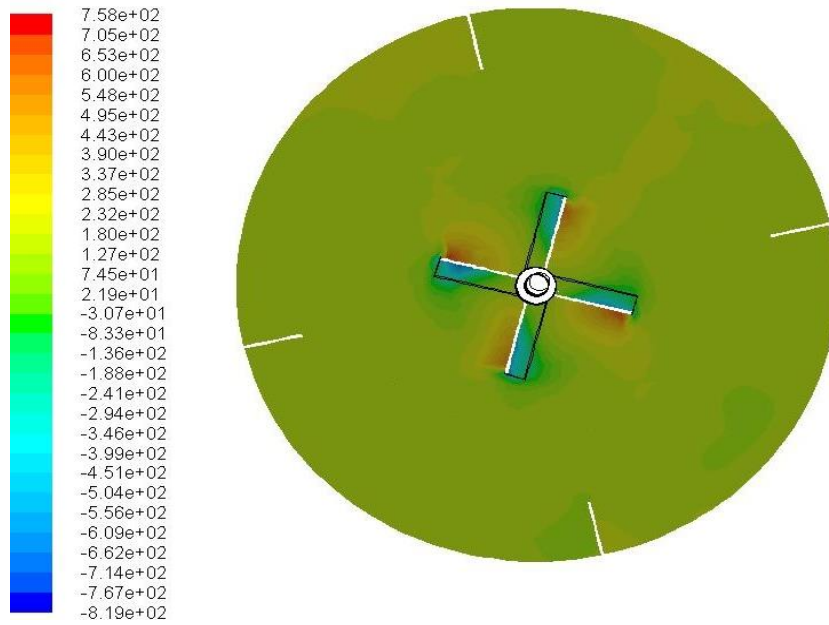


Figure 30. Horizontal cut of the vessel in the plane of the impeller. Static pressure contours. (Less dense model)

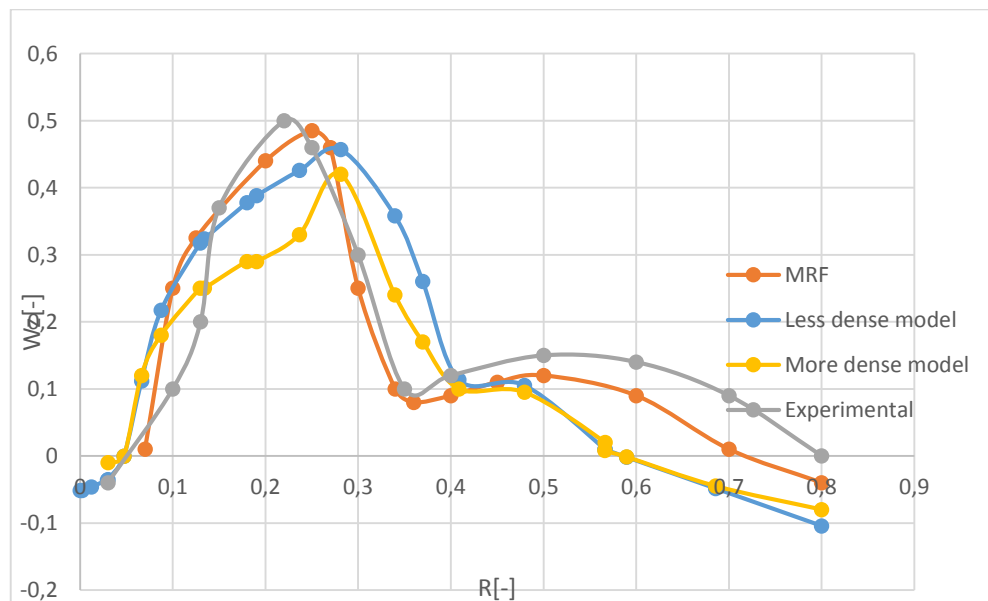


Figure 31. . Comparison of velocity profile of experimental, MRF and CFD simulations, experimental data from [12]

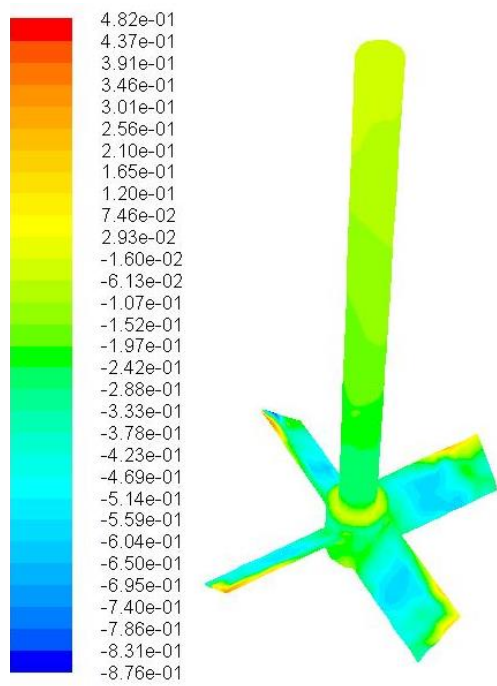


Figure 32. Cut turbulence intensity (m/s). (Less dense model)

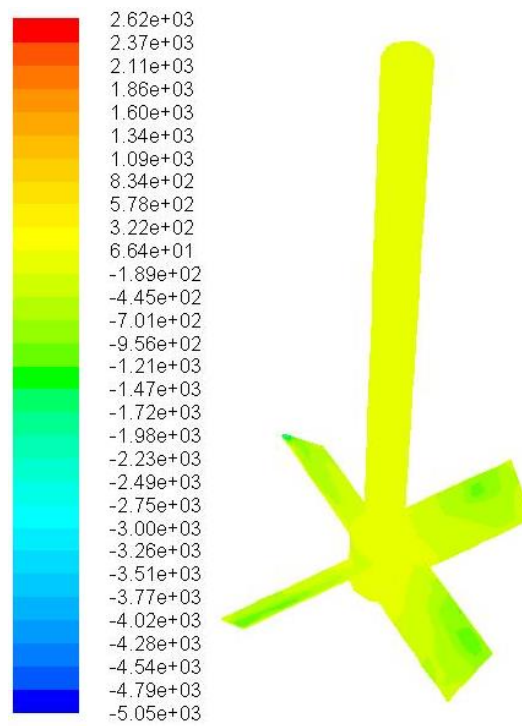


Figure 33. Contours of shear stress. (Less dense model)

The Figure 31 shows the simulated time averaged radial axial velocities for both less and more dense models. Velocity profiles from the models are compared with MRF method profile from [10] and experimental data for four blades impeller [12]. Experimental data are done at same radial distances in a $T = 300$ mm vessel and for the impeller rotating at 300 rpm. There are direct geometrical similarity between four blades from experiment and four blades geometry that are used in this report. The results does not show a good agreement between experimental, MRF, and simulation data. However, the pattern of the velocities shows to be similar.

6. CONCLUSION

In this master thesis, the application Large Eddy Simulation to predict turbulence flow in a stirred tank was investigated. The impeller and tank's geometry was simplified in the simulation. The flow field, flow number, and power number were predicted by using the program (ANSYS-Fluent 15). The numerical results were compared with the experimental data obtained from the literature. A good agreement was found between numerical flow number, and power number with experimental data. In addition, good prediction for a typical flow pattern in a stirred tank. Was found, the velocity profiles in the axial direction were not in an excellent agreement with the experimental data.

The results for the optimal mesh with more dense model showed less precision than the model with less amount of mesh elements. The reason was the calculation supposed to takes months of calculation, and the software were cancelled before the convergence reaches stability, due to time constrains. The computation time for LES approach dramatically rise with increasing number of elements and the duration of calculation was estimated in months, which was expected.

List of notation

A: area, [m²]
bi: Amount of baffles [-]
C: Impellers height from bottom of the tank [m]
D: Diameter of the impeller, [m]
H: Water level, [m]
N: Impeller rotating speed, [Revs*s⁻¹]
 $N_{Qp,exp}$: Flow rate number from experimental [-]
 $N_{Qp,comp}$: Flow rate number from computer [-]
 N_Q : Flow number, [-]
p: Pressure, [Pa]
P: power, [W]
 P_0 : power number [-]
Q: Mas flow rate/pumping capacity, [kg*s⁻¹]
r: Radius, [m]
 R^* : Dimensionless radius, [-]
 Re : Impeller Reynolds number, [-]
T: Vessels outer diameter, [m]
 \overline{Wz} : Ensemble-average mean velocity, [m*s⁻¹]
 Wz^* : Dimensionless velocity, [-]

Greek letters

ρ : liquid density, [kg*m⁻³]
 μ : liquid viscosity, [Pa s]
 ε_l : dissipation associated with the large scales eddies, [m²*s⁻³]

 ε : turbulent dissipation rate, [m²*s⁻³]
 ε_{sgs} : dissipation of the sub-grid scales eddies, [m²*s⁻³]
 Γ : torque, [N*m]
 Γ_l : molecular diffusivity, [m²*s⁻¹]

Γ_t : eddy diffusivity, [m^2s^{-1}]

σ_t : turbulent Schmidt number

μ_t : turbulent viscosity, [$\text{Pa}\cdot\text{s}$]

α : Blade angle [-]

k- ϵ : k-epsilon turbulence model

Subscripts

i, j: coordinate directions

t: turbulent

BC: Boundary condition

CFD: Computer fluid Dynamic

LDA: Laser Doppler Velocimetry

LES: Large Eddy Simulation

MRF: Moving Reference Frame

PIV: Particle Imaging Velocimetry

RANS: Reynolds Averaged Navier-Stokes

RNG: Re: normalization

rpm: Revolutions per minute

SG: Sliding Grid

SM: Sliding Mesh

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