

CFD modelling of single and multiphase flow in a stirred tank reactor

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Synopsis

The primary aim of this project is to validate the single-phase simulation in stirred tank reactor with the experimental results conducted by Wu and Patterson [1] using OpenFOAM and understand the flow characteristics due to the Rushton turbine. simpleFoam is a steady incompressible solver which is used in this study. The normalized radial and tangential velocities by the tip velocity are compared with [1]. A Multiple Reference Frame(MRF) model is employed to simulate the rotating impeller blade of the Rushton turbine and the $k-\epsilon$ turbulence model is used for the study.

1 Introduction

Stirred tanks are widely used for mixing various chemicals in the chemical, oil and gas, metallurgical and pharmaceutical industries. The performance of stirred tank depends on the type and size of the impeller, the aspect ratio of the vessel, baffles, impeller clearance, etc [2]. Among the type of impellers, the Rushton turbine is one of the popular turbines which is known for good mixing in low-viscosity fluid. The flow leaves the impeller in the radial and tangential direction of the Rushton turbine. The flow again recirculates back to the impeller region which improves dispersion and mixing of substances. Computational Fluid Dynamics(CFD) has been used to extract detailed information about flow characteristics in stirred tank reactors. Since this is a single-phase simulation, it is less complex than a multiphase simulation. Single-phase contains fluid having a single homogenous phase. The MRF model and $k-\epsilon$ turbulence model are used to understand the flow in stirred tank reactor [3, 4]. In this current work, the MRF model and $k-\epsilon$ turbulence model are employed to simulate the stirred tank reactor using OpenFOAM.

2 Governing Equations and Models

The incompressible solvers consist of kinematic pressure which is the ratio of static pressure and density of the fluid. The incompressible Navier Stokes equation is given by:

$$\nabla \cdot (UU) = -\frac{1}{\rho} \nabla p + \nabla \cdot (\nu \nabla U) \quad (1)$$

The Multiple Reference Frame (MRF) enables the simulation of rotating parts without the need for rotating mesh. The rotating zone must be a cylinder in shape to utilize the MRF model. The main advantage of MRF in regard to the sliding mesh technique is it has a lower computational cost. For Multiple Reference Frames (MRF), the Navier-Stokes equation will become:

$$\nabla \cdot (UU_r) = -\nabla p + \nabla \cdot (\nu \nabla U) - \Omega \times U \quad (2)$$

The additional source term needs to be accounted for in the rotating zone.

With the mean fluctuating velocity set to zero, RANS equations are time-averaged Navier Stokes equations. The stress tensor responsible for energy loss is known as $\tau_{ij} = -\overline{\rho u_i u_j}$. Turbulence modeling is applied to deal with the closure problem because of τ_{ij} . The most popular RANS turbulence modeling techniques use two-equation models, which use the two parameters; turbulence kinetic energy and turbulence length scale. Various models, such as SKE, SKO, SST $k-\omega$, etc., are used to overcome the closure problem that RANS equations produce.

$$k = \frac{3}{2}(u_m I)^2 \quad (3)$$

$$\epsilon = C_\mu \frac{\rho k^2}{\mu} \left(\frac{\mu_t}{\mu} \right)^{-1} \quad (4)$$

I = turbulent intensity
 $\left(\frac{\mu_t}{\mu} \right)$ = eddy viscosity ratio.

In order to mimic the mean flow characteristics under turbulent flow circumstances, the $k-\epsilon$ model, a two-equation model, is frequently utilized. It is composed of two transport equations (PDEs) that take into consideration the convection and diffusion of turbulence, in addition to conservation equations. The two conveyed variables are turbulent dissipation rate (ϵ), which describes the rate at which turbulent kinetic energy dissipates, and turbulent kinetic energy (k), which describes the energy in turbulence. In OpenFOAM, the turbulent kinetic energy(k) and turbulent dissipation rate(ϵ) are both divided by the density(ρ). Hence, all the terms which consist of viscosity are kinematic viscosity(ν) rather than dynamic viscosity(ϵ). The k and ϵ transport equations are:

$$\frac{\partial \rho k}{\partial t} + \nabla \cdot (\rho U k) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k + P_b - \rho \epsilon + S_k \quad (5)$$

$$\frac{\partial \rho \epsilon}{\partial t} + \nabla \cdot (\rho U \epsilon) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \nabla \epsilon \right] + C_1 \frac{\epsilon (P_k + C_3 P_b)}{k} - C_2 \rho \frac{\epsilon^2}{k} + S_\epsilon \quad (6)$$

The model coefficients in these equations are: $C_{1\epsilon} = 1.44$, $C_{2\epsilon} = 1.92$, $C_\mu = 0.09$, $\sigma_k = 1$ and $\sigma_\epsilon = 1.3$

3 Simulation Procedure

3.1 Geometry and Mesh

A detailed discussion on the creation of geometry and its meshing. The software used for creating the geometry and its mesh needs mentioning. Mention, if any, the number of blocks, refinement/-grading in the mesh, etc.

The geometry for the single-phase stirred tank simulation was taken from the [3] which contains a 15 cm diameter cylindrical tank with four baffles equally spaced to each other that is agitated by a six-bladed Rushton turbine impeller. The disc and blades in an impeller are modeled with infinitely thin surfaces.

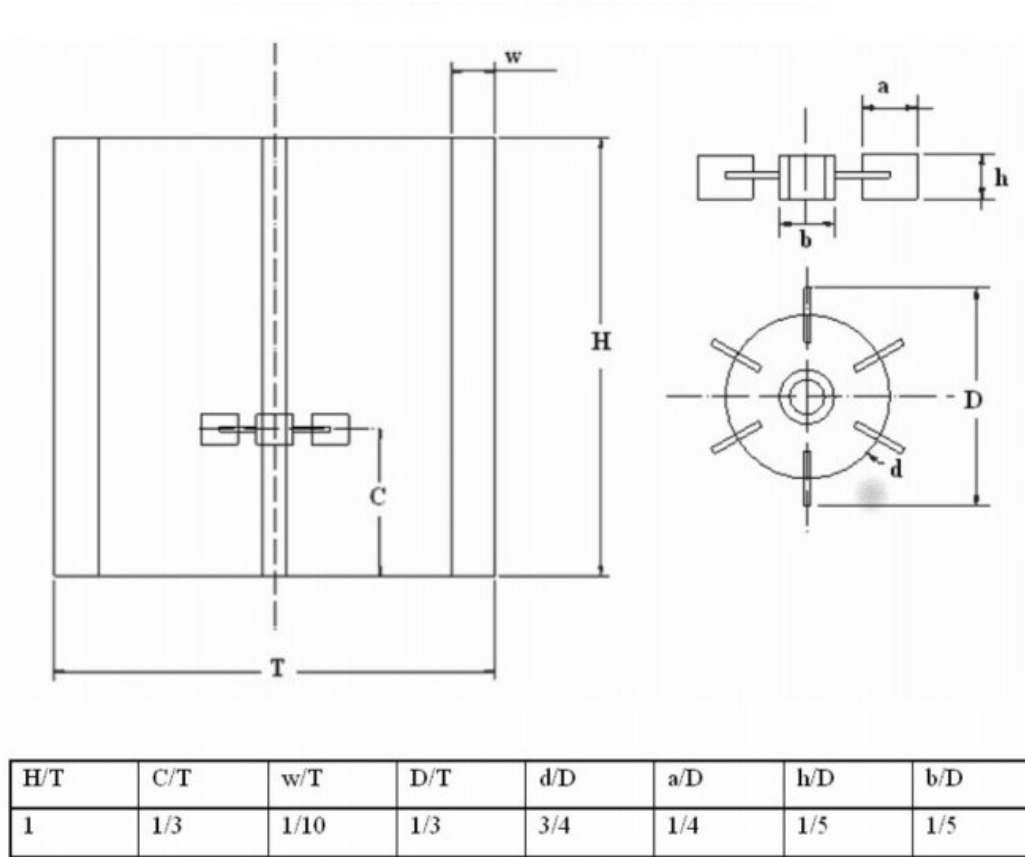


Figure 1: Rushton turbine impeller and stirred tank configuration from [3]

The CAD model of the stirred tank and Rushton turbine was made in CATIA V5. The meshing of the whole computational domain was performed using blockMesh and snappyHexMesh which are built-in mesher in OpenFOAM. blockMesh is a comprehensive software tool used for defining and meshing geometries, which don't require the import of CAD files of geometry. To create blockMesh, the geometry, patch information, and number of cells are defined in blockMeshDict. The assignment of local vertex numbers is a crucial aspect when defining a block in mesh generation in blockMeshDict. The initial section of blockMeshDict typically consists of a series of vertices,

which form the foundation for constructing the blocks. A block is specified by a list of eight vertices that must be arranged in a manner that corresponds to the local vertices. Moreover, edges are numbered and possess a specific direction.

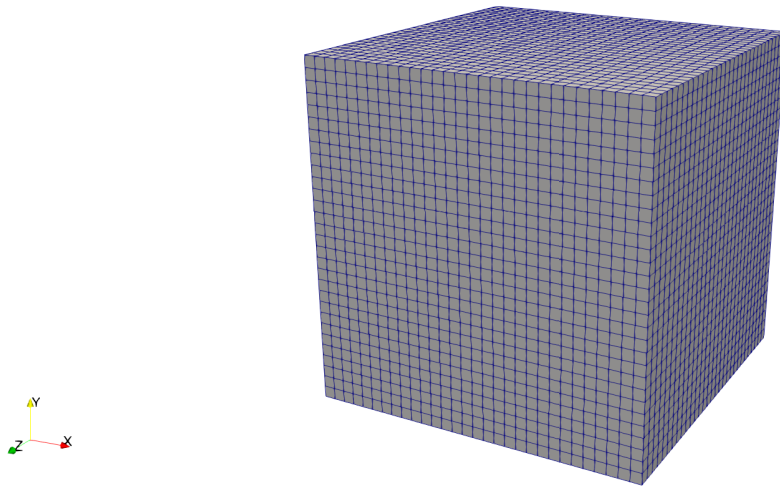


Figure 2: Creation of background mesh using blockMesh

snappyHexMesh is a meshing tool designed to generate meshes for the surrounding space of a triangulated surface, such as an STL surface mesh. It is specifically used in conjunction with blockMesh, as it relies on a background mesh for its operation. It generates mesh doing steps that include castellation, snapping, and layer addition. However, layer addition was disabled in this case as it requires more time. It generates high-quality structured mesh as can be seen in Figure(3).

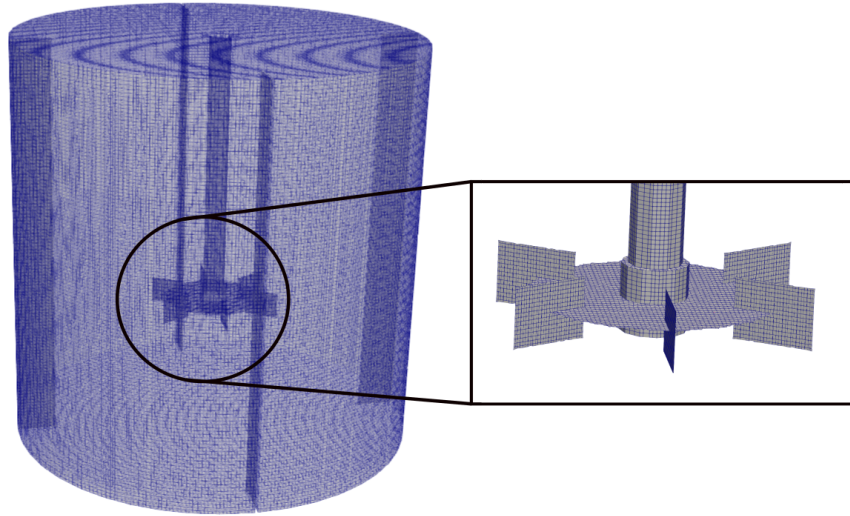


Figure 3: structured mesh generated using snappyHexMesh

In Figure (4), the slice of internal mesh is shown where more refined mesh can be observed near the blade of an impeller. The cellMRFzone is cylindrical and has 16cm height and 26mm radius [5]. It encloses the blade and disc of an impeller completely. This dimension can be defined in snappyHexMeshDict.

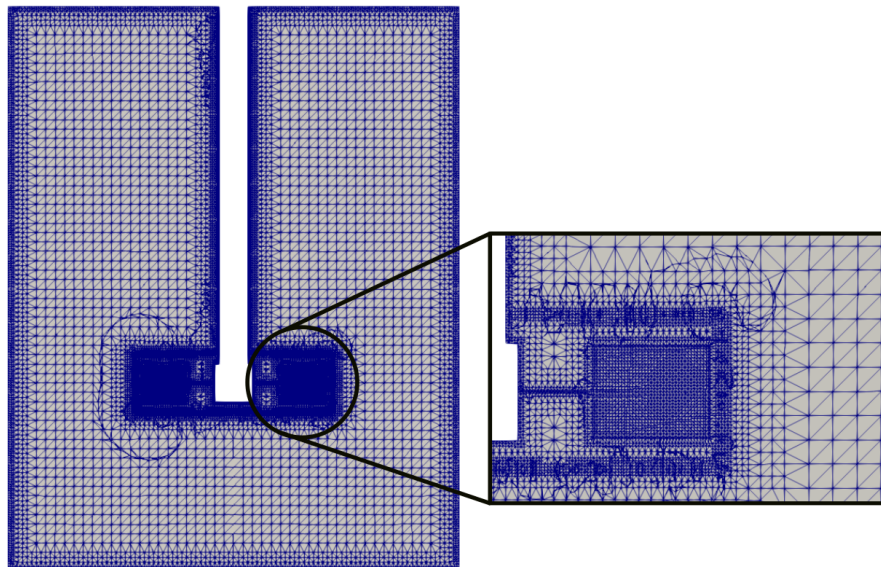


Figure 4: slice of computational grid

3.2 Initial and Boundary Conditions

To accurately represent the real-world issue in the case study, a good boundary condition is essential. Water is used as working fluid in the tank with density(ρ)=997 kg/m³ and dynamic viscosity(μ) = 0.00089 kg/ms. The Reynolds number of an impeller was 40000.

Patch	Condition	Value ($m s^{-1}$)
vessel	fixedValue	(0, 0, 0)
impeller	fixedValue	(0, 0, 0)

Table 1: Boundary Condition for U

Patch	Condition	Value ($m^2 s^{-2}$)
vessel	zeroGradient	-
impeller	zeroGradient	-

Table 2: Boundary Condition for p

Patch	Condition	Value ($m^2 s^{-1}$)
vessel	nutkWallFunction	-
impeller	nutkWallFunction	-

Table 3: Boundary Condition for nut

Patch	Condition	Value
vessel	epsilonWallFunction	-
impeller	epsilonWallFunction	-

Table 4: Boundary Condition for ϵ

Patch	Condition	Value ($m^2 s^{-1}$)
vessel	kqRWallFunction	-
impeller	kqRWallFunction	-

Table 5: Boundary Condition for k

3.3 Solver

simpleFoam solver is used for the simulation of a single phase in stirred tank reactors. simpleFoam is a steady-state incompressible turbulent flow solver which utilizes the SIMPLE(Semi-Implicit Method for Pressure Linked Equations) algorithm). The SIMPLE algorithm first predicts the velocity, corrects the pressure and velocity, and then solves turbulent quantities which continue until convergence criteria are met. The unknown quantities are U_x , U_y , U_z and p. p is the kinematic

pressure which is the ratio of static pressure and density of the fluid. Since the momentum equation is highly non-linear, an iterative algorithm approach is used to solve the pressure-velocity coupling problem.

$$MU = -\nabla p \quad (7)$$

Equation (7), gives the linear algebraic form of the momentum equation which is also known as momentum predictor. M is the square matrix with known quantities that are obtained using the Finite-Volume approach in OpenFOAM.

$$AU - H = -\nabla p \quad (8)$$

The matrix M is decomposed into diagonal (A) and off-diagonal (H) matrix as in equation (8) Now, the velocity equations are solved using the initial conditions and then needs to satisfy the continuity equation.

$$\nabla \cdot (A^{-1} \nabla p) = \nabla \cdot (A^{-1} H) \quad (9)$$

Thus, the continuity equation gives an equation for the pressure term which when solved gives the pressure field that can be used to correct the velocity field, so that it satisfies the continuity equation. The corrector loop is repeated until the desired residual is achieved for a single iteration.

Step 1: Check the residual tolerance criteria of pressure, velocity, and turbulent quantities

Step 2: Predict the velocities using momentum predictor

Step 3: Correct the pressure and velocities

Step 4: The turbulence-related fields are then corrected.

Step 5: Go to step 1

```

SIMPLE
{
    nNonOrthogonalCorrectors 1;
    consistent yes;
    pRefCell 0;
    pRefValue 0;
    residualControl
    {
        U 1e-4;
        p 1e-3;
        "(k|epsilon|omega)" 1e-4;
    }
}

relaxationFactors
{
    equations
    {
        U 0.1;
        p 0.1;
        "(k|omega|epsilon)" 0.1;
    }
}

```

```
}
}
```

Residual control is used to monitor the convergence of the solution. The residuals represent the difference between the calculated values and the values from the previous iteration and are used as a measure of the accuracy of the solution. Here, the solution is converged when the residual of pressure is below $1e-3$ and below $1e-4$ for velocity and turbulent parameters fields.

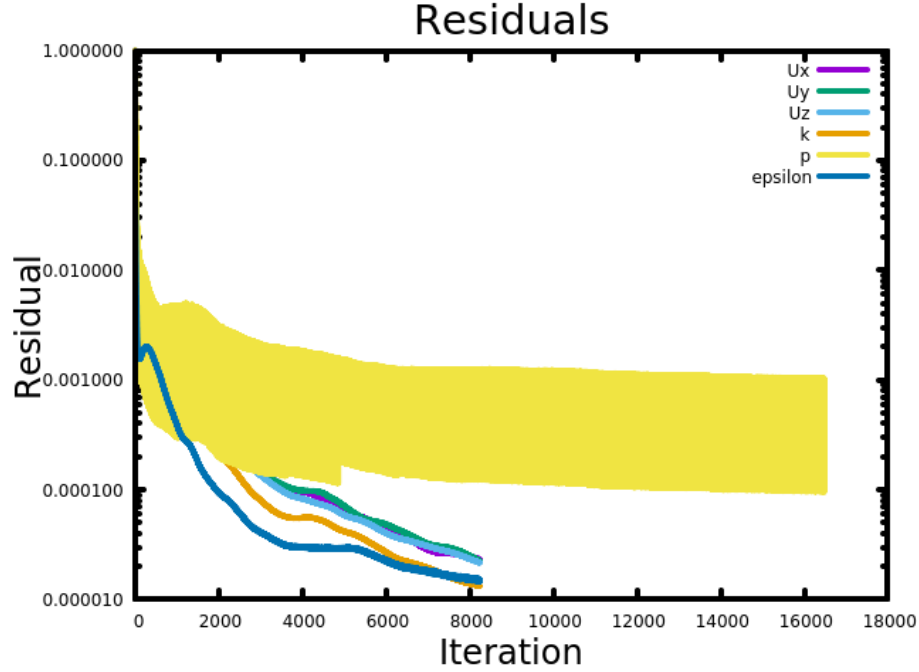
Similarly, non-orthogonal correctors are used in simulations where non-orthogonality exists between the cell faces of a computational mesh. Non-orthogonality refers to the angle between the cell faces not being exactly 90° . Non-orthogonal meshes are common in many real-world simulations and can result in inaccuracies in the results obtained from simulations. To overcome this issue, OpenFOAM provides several non-orthogonal correctors that solve the pressure-velocity coupling problem in non-orthogonal meshes and help to ensure that the simulation results are accurate. In the present study, the maximum non-orthogonality of the mesh was around 65.19° and also to minimize computational time only 1 corrector was used in the simulation.

In CFD, relaxation factors are used to accelerate the convergence of the solution. The relaxation factors control the rate at which the pressure, velocity, turbulence parameters, and C fields are updated in each iteration. In general, a relaxation factor of 1 means that the variable is updated completely in each iteration, which can result in fast convergence or even instability. A relaxation factor less than 1.0 means that the update is less aggressive, and can help to accelerate convergence. However, too small of a relaxation factor can result in slow convergence. In this simulation, we used a relaxation factor of 0.1 for pressure, velocity, and remaining fields to obtain a stable solution.

Different interpolation schemes are used to estimate the value of fields at the face center from the value stored at the centroid of the cell. linearUpwind scheme is used as the divergence scheme which is second order upwind scheme.

4 Results and Discussions

The steady-state simulation was performed using the SIMPLE algorithm for the $k-\epsilon$ turbulence model. Residuals are parameters to monitor the behavior of the numerical process. It gives information whether the solution is converging or diverging. The convergence criteria were specified in terms of residuals which were specified to be 10^{-3} for pressure and 10^{-4} for other fluid flow properties.

Figure 5: Residual plot of k- ϵ model

4.1 Mesh Independence Study

Determining the optimal amount of mesh components is essential to correctly and effectively tackle a particular problem. The outcomes were compared between three distinct mesh configurations that were built. The number of cells is represented by M1, M2, and M3. The mesh configuration along with the number of cells are tabulated in Table(6). The ratio of radial velocity and tangential velocity with respect to the tip velocity of the blade against $2z/w$ is plotted for different numbers of grids. The value of normalized radial and tangential velocities for the corresponding mesh configuration are within 5 %. Mesh independence is achieved when refining the mesh doesn't improve the accuracy of the solution [6]. After thoroughly evaluating the three mesh options for use, the M1 mesh was ultimately chosen for further analysis which is cost-effective.

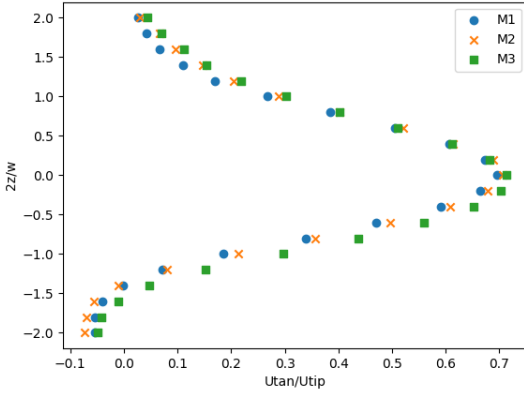


Figure 6: Normalized tangential velocity plot for different grids

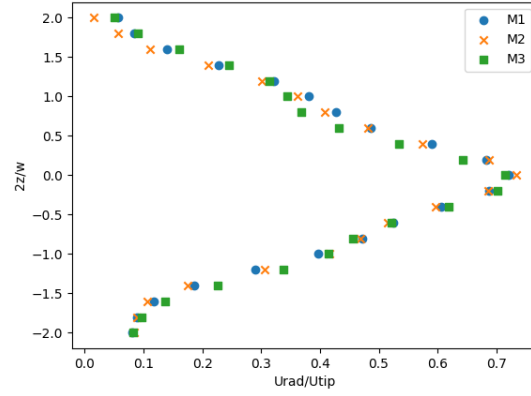


Figure 7: Normalized radial velocity plot for different grids

Mesh configuration	Number of cells
M1	391440
M2	715880
M3	1682561

Table 6: Mesh Sensitivity Analysis

4.2 Validation

The velocities (radial, tangential) normalized by the tip velocity of the blade are independent of the velocity of the blade and size of the tank for geometrically similar tanks [1, 7]. Hence, the normalized radial and tangential velocities obtained from the simulation are compared with the experimental results of [1] as shown in Figure(8) and Figure(9). The ratio of radial and tangential velocities with respect to the tip velocity of the blade is plotted against $2z/w$ where 'z' represents the axial height from the blade disc and 'w' represents the height of the blade. Both simulated normalized radial and tangential velocities plots are flatter than the experimental results. This is due to the difference in thickness of the baffle, the actual geometry of the impeller, and the inability of the $k-\epsilon$ turbulence model to accurately simulate the flow near impeller region [4]. The numerical errors are the cause of this poor prediction [3].

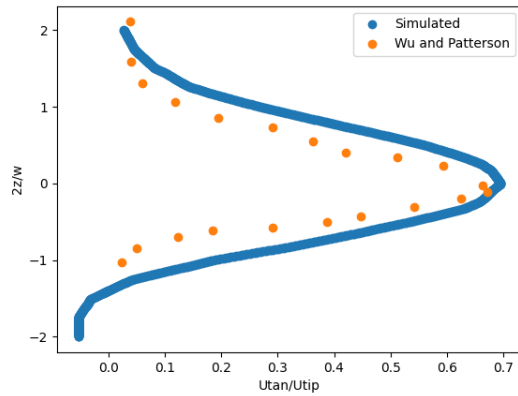


Figure 8: Normalized tangential velocity plot

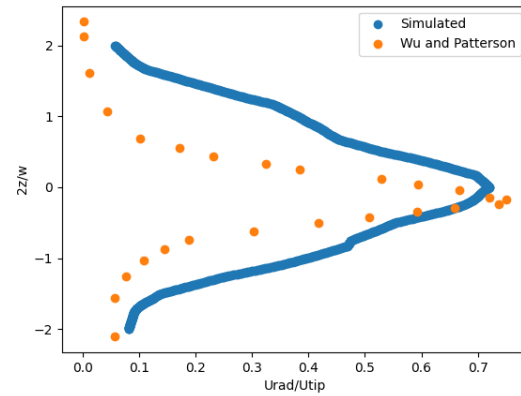


Figure 9: Normalized radial velocity plot

The velocity contour, pressure contour, and velocity vector plot are shown in Figure(10), Figure(11), and Figure(12) respectively. In the vector plot, it can be clearly seen the flow leaves the impeller in radial and tangential directions which again recirculate back to the impeller region. The radial and tangential velocity contour is observed in Figure(13) and Figure(14) respectively.

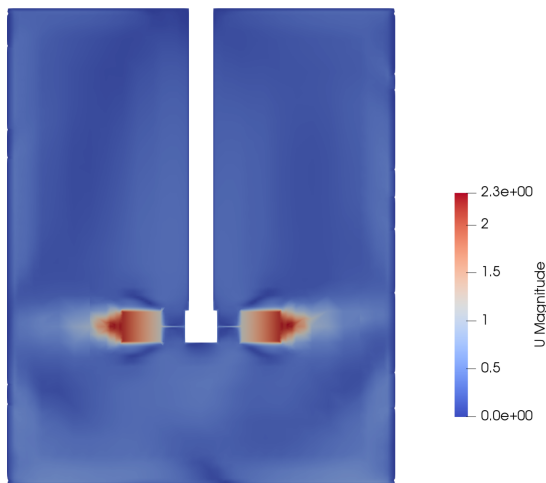


Figure 10: velocity contour plot

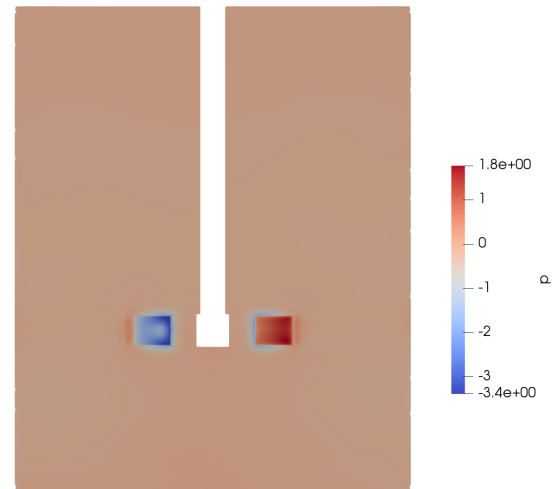


Figure 11: pressure contour plot

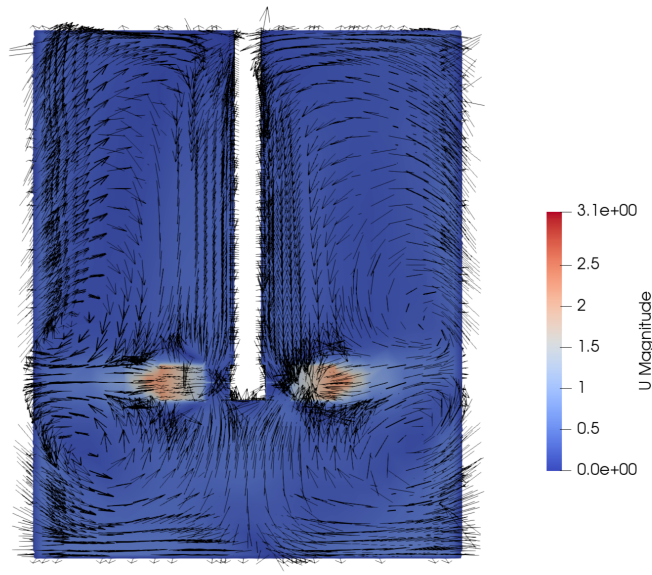


Figure 12: velocity vector plot

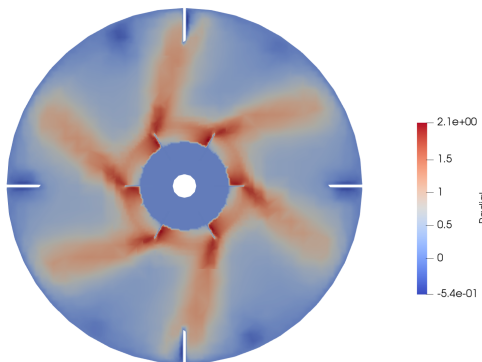


Figure 13: Radial velocity

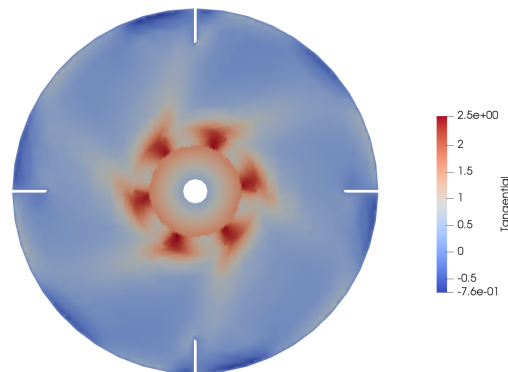


Figure 14: Tangential velocity

5 Conclusion

The present study investigates the flow in stirred tank reactor using OpenFOAM. The numerical results obtained from the simulation have a good agreement with the experiment results available in the literature. The normalized radial and tangential velocities aren't strongly affected by the number of cells provided that the mesh is not too coarse.

6 Acknowledgement

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