CFD5 Second Assignment

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Abstract

This is the second assignment in the Edinburgh University CFD 5 course, in which a modified CTP (Chemical Transfer Partnership) ChemReactor CR60 is simulated using Starccm+.

Contents

1 Interpretation of the Assignment Question

The remit states:
"*You are required to perform a CFD simulation of the inside the reactor and produce a report (of no more than 6 pages A4, including figures) summarising your results for the technical director of ECI plc.*"

From this it has been inferred that the most likely concerns of the technical director must be anticipated and addressed. From the literature referenced in the remit a number of objectives have been deduced (Dickey et al. (2004) and Li et al. (2005)):

- Macro and micro mixing performance
- Vorticity
- Temperature distribution – Although not mentioned in the literature it was thought that temperature distribution may be of interest.

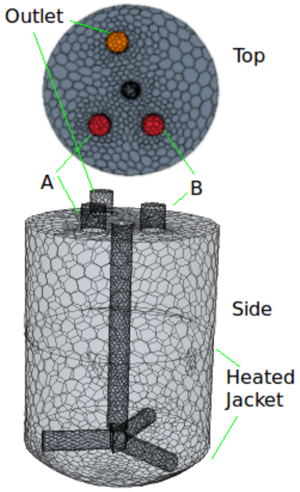

Figure 1: Top and side view of the reaction vessel geometry.

Another frequently discussed issue in the literature is pumping efficiency– normalised parameters such as the impeller power number are used to describe this. However since the impeller is not rotating such a number is meaningless.

The meshed model of the reaction vessel is given in figure 1. The DN 400 reaction vessel is 477mm tall. The DN 50 inlet and outlet pipes are also depicted. Since no mention was made of a baffel, it has been assumed that one has not been installed. Inlet conditions for reagent A were 2.5 L/s and 90 degrees C, for reagent B 1 L/s and 10 degrees C. Although a turbulent velocity profile can be easily be imported in Starccm+ plug flow was assumed. Approximate scaled dimensions from Li et al. (2005) were used for the impeller. As suggested in the remit the fluids have been assumed to be water with a dynamic viscosity, ν of $10^{-6} m^2/s$ and a density of $1000 kg/m^3$.

2 Methodology

In Starccm+ it is possible to produce a variety of different meshes by selecting from a range of meshing models available in the program. It was found that only the polyhedral meshing model was suitable for the complex geometry of the reaction vessel. The free surface was treated as a slip wall, since the alternative volume of fluid method would required more processing power without providing much further information. An unsteady simulation was run using carefully selected settings to provide accurate results whilst maintaining a fast convergence rate. These settings are surmised in the appendix.

3 Results

Three grids were used for a grid convergence study, using the Octave code by Ulerich (2009), the results are presented in figure 3. By using the Grid Convergence Index (GCI) method of presenting the results as recommended by Celik et al. (2008), it can be seen that a grid converged solution was obtained.

Grid	Spacing (m)	Outlet Temp (K)	GCI (%)
1	0.01	342.1	-
2	0.02	341.2	1.15
3	0.04	340.5	0.898

Figure 2: Grid convergence study.

It was decided that presenting the results in the form of scalar or vector scenes provided an intuitive means to assess the performance of the reaction vessel. For this 5 plane sections where used. Two sections where obtained by making two perpendicular cuts across the reaction vessel axis. Another three planes were created by making cuts along the length of the vessel as shown in figure 3.

To check the time dependent nature of the flow scenario an animation was made in Starccm+. From the animation it was clear that the flow could have been assumed to be quasi-steady, saving on computational cost.

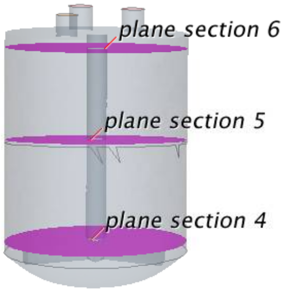

Figure 3: Position of three cuts made on the reaction vessel used in the scalar scenes in this report.

3.1 Macro Mixing

An understanding of the macro mixing capabilities can be attained upon examining the streamlines in figure 4. The slower reagent B is drawn into the flow path of reagent A and recirculates along the walls of the reaction vessel.

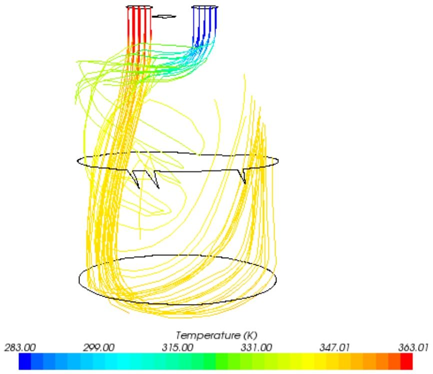

Figure 4: By seeding the inlets A and B streamlines where produced which show the macroscopic mixing of the two reagents. Also the streamlines have been coloured according to their temperature. Once the reactants reach the bottom of the reaction vessel a thermal equilibrium of around 70 degrees C is reached.

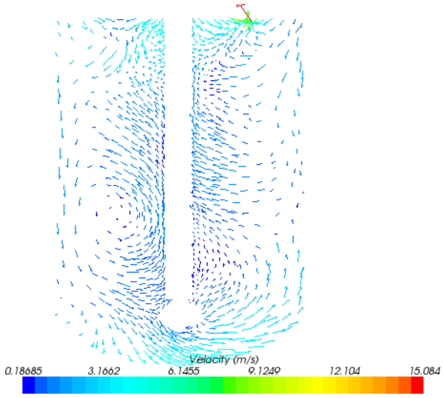

Figure 5: A cross-section cut of the reaction vessel, displaying a velocity vector scene.

Vortex structures can be seen in the cross-sections in figures 6 and 7, with the greatest flow rates around the impeller blades. In figures 7, 8 and 9, vortices are present mostly in the upper regions of the vessel.

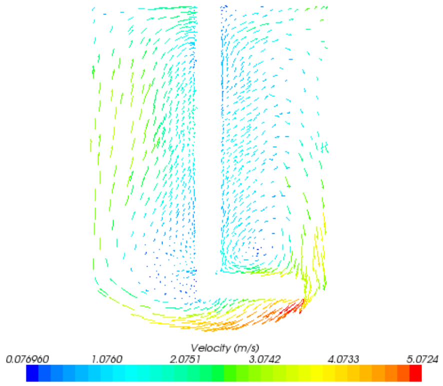

Figure 6: A cross-section cut of the reaction vessel, displaying a velocity vector scene. A maximum flow rate of circa 5 m/s is reached at the blade tip.

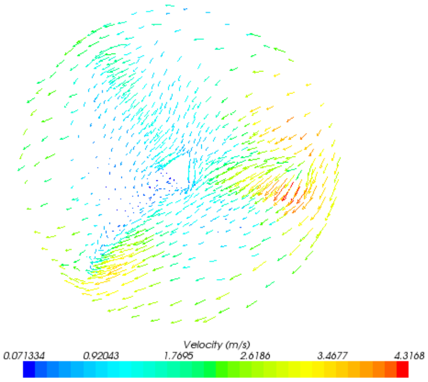

Figure 7: Plane 4 cut of the reaction vessel, displaying a velocity vector scene.

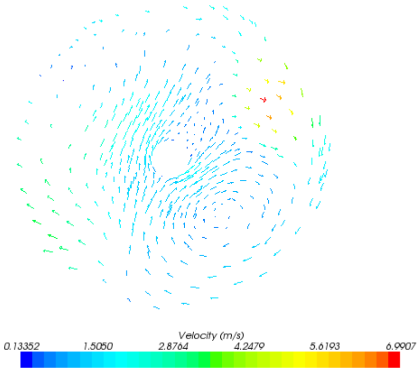

Figure 8: Plane 5 cut of the reaction vessel, displaying a velocity vector scene.

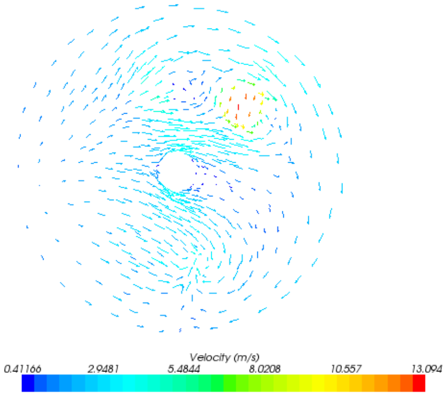

Figure 9: Plane 6 cut of the reaction vessel, displaying a velocity vector scene.

3.2 Micro Mixing

The field function vorticity was used to assess the micro mixing levels. In figures 10 and 11 it can be seen that the mean vorticity is around 100 /s. At the inlet and around the blades the vorticity is greater at around 120 /s. In the uppermost plane the greatest amount of vorticity is present, located at inlet B (see figure 14). By examining figures 12 and 13 it is apparent that the vorticity created by the inlet is dispersed nearing the bottom of the vessel and replaced by the vorticity created by the impeller blades.

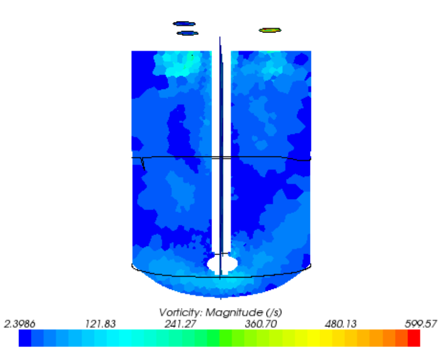

Figure 10: A cross-section cut of the reaction vessel, displaying the vorticity.

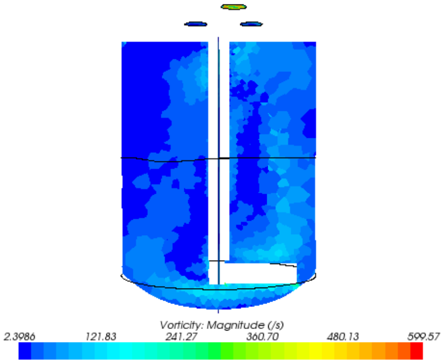

Figure 11: A cross-section cut of the reaction vessel, displaying the vorticity.

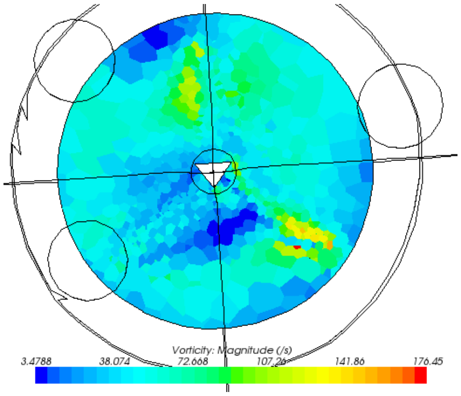

Figure 12: Plane 4 cut of the reaction vessel, displaying the vorticity.

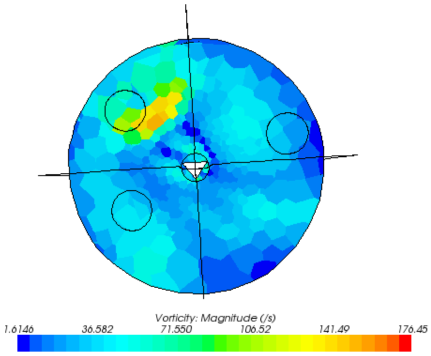

Figure 13: Plane 5 cut of the reaction vessel, displaying the vorticity.

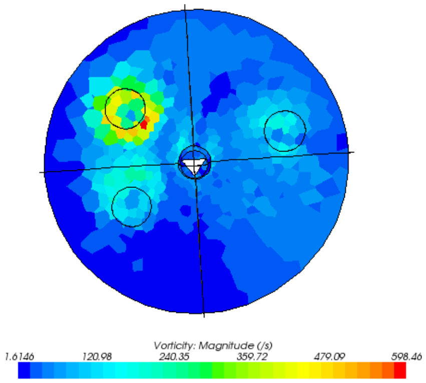

Figure 14: Plane 6 cut of the reaction vessel, displaying the vorticity.

3.3 Thermal Mixing

An overview of thermal behaviour of the reaction vessel at the walls can be seen in figure 15. Cuts of the reaction vessel in figures 15 and 16, reveal an even temperature distribution. However on the other cross-section and planes 4, 5, 6 this is not the case (figures 17, 18, 19 and 20). The largest temperature gradient can be seen in the middle plane (plane 5).

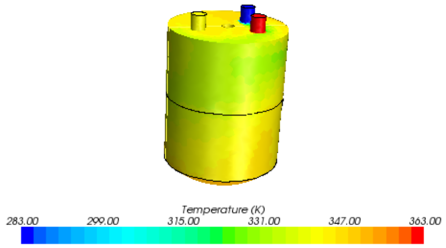

Figure 15: An overview of the thermal distribution near the walls. It can be seen that the temperature is a fairly even 70 degrees C.

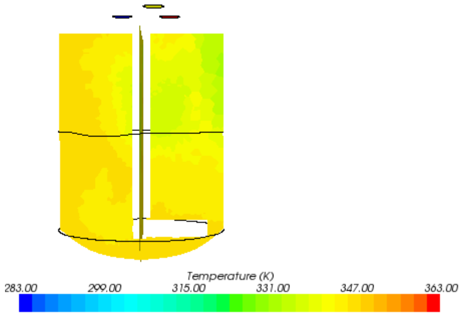

Figure 16: A cross-section cut of the reaction vessel, displaying the temperature distribution.

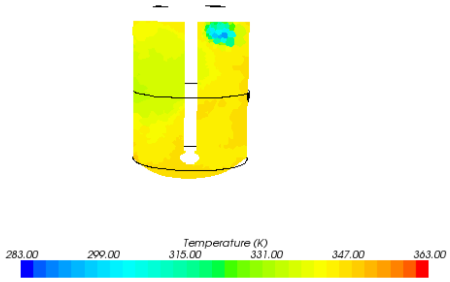

Figure 17: A cross-section cut of the reaction vessel, displaying the temperature distribution.

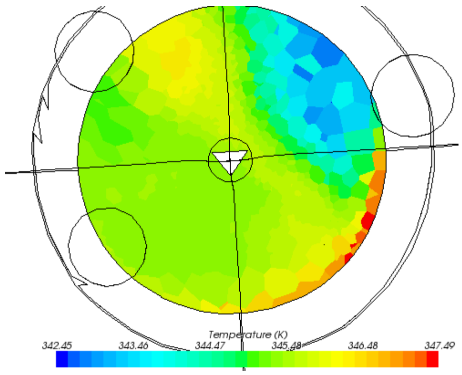

Figure 18: Plane 4 of the reaction vessel, displaying the temperature distribution.

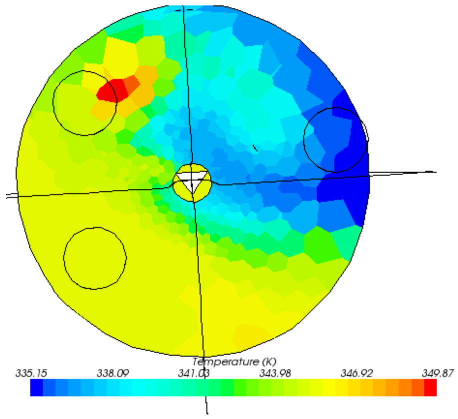

Figure 19: Plane 5 of the reaction vessel, displaying the temperature distribution.

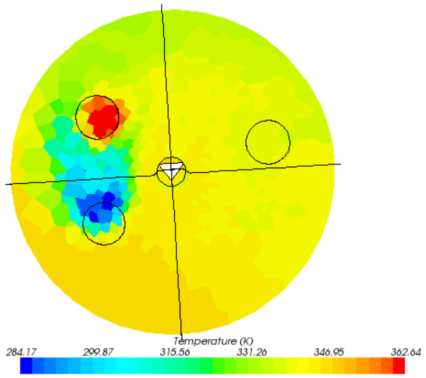

Figure 20: Plane 6 of the reaction vessel, displaying the temperature distribution.

3.4 Validation

Unfortunately there has not been any published experimental work on reaction vessels with a stationary impeller. However in Li et al. (2005) it was found that the using the program CFX, the Shear-Stress-Transport model in combination with an unstructed mesh produced accurate results without arbitrary parameter tuning. Although Starccm+ and the k-ϵ model was used instead this still indicates that the problem is well defined. By conducting a few experiments across the spectrum of scenarios it could be possible to validate the CFD results. Depending on the level of validation required, the experiments could range from inexpensive flow visualization using ink streaks to high resolution particle image velocimetry.

4 Conclusion

A grid converged solution for the given scenario was found. Due to a lack of literature on reaction vessels in which the impeller is stationary it has not been possible to validate the results in this report and therefore experimental research shall be required to do this. Microscopic, macroscopic and thermal mixing is present. These results have been presented visually for interpretation by the chemical engineering department and the technical director at ECI plc.

References

Celik, I. B., Ghia, U., Roache, P. J., Freitas, C. J., Coleman, H. and Raad, P. E. (2008). Procedure for estimation and reporting of uncertainty due to discretization in cfd applications, *Journal of Fluids Engineering* **130**(7): 078001.
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Dickey, D. S., Bittorf, K. J., Ramsey, C. J. and Johnson, K. E. (2004). Understand flow patterns in glass-lined reactors, *Chemical Engineering Progress* **100**(11): 21 – 25.

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Ulerich, R. (2009). richardson.m. Accessed 120111.
URL: *http://www.mathworks.com/matlabcentral/fileexchange/24388*

List of Figures

A Appendix

Summary of Settings Used

Setting	**Action/Justification**
Continua/Regions	
Fluid, water	
Constant density	Water is incompressible.
Segregated flow	Alternative would be coupled–not necessary for low Mach number flows.
Unsteady	It was assumed that the flow was unsteady, although only small time dependent flow patterns were detected.
Timestep	A timestep of 0.5s was used. This was thought to be sufficiently small. For higher time resolution a smaller timestep would be required.
Inner Iterations	125 inner iterations were used as this proved to provide the fastest convergence rate.
k-ε turbulence model	Flow in reaction vessels are turbulent. The alternatives were k-ω, which is suitable for higher Re and Spalart Almar which is only very useful for wings.
Two layer all y+ wall treatment	This is the only wall treatment available in Starccm+, for the k-ε turbulence model.
Initial pressure	A pressure of $0Pa$ was assumed at the inlets, $0Pa$ at the exit and the reference pressure was set to 10^5Pa.
Turbulence specification	Intensity + viscosity ratio of 0.01 and 10 used respectively, these values are simply estimates.
Other	For any of the other settings not mentioned the default program settings were used.

Table 1: Summary table of the settings I used in my simulations