

## SCREENING OF OPTIMIZATION PARAMETERS FOR MIXING PROCESS VIA CFD

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### ABSTRACT

*In this study, the numerical simulation in a mixing vessel agitated by a six bladed Rushton turbine has been carried out to investigate the effects of effective parameters to the mixing process. The study is intended to screen the potential parameters which affect the optimization process and to provide the detail insights into the process. Three-dimensional and steady-state flow has been performed using the fully predictive Multiple Reference Frame (MRF) technique for the impeller and tank geometry. Process optimization is always used to ensure the optimum conditions are fulfilled to attain industries' satisfaction or needs (ie; increase profit, low cost, yields, etc). In this study, the range of recommended speed to accelerate optimization is 100, 150 and 200rpm respectively and the range of recommended clearance is 50, 75 and 100mm respectively for dual Rushton impeller. Thus, the computer fluid dynamics (CFD) was introduced in order to screen the suitable parameters efficiently and to accelerate optimization.*

### ABSTRAK

*Dalam kajian ini, simulasi berangka dalam sebuah mangkuk campuran yang digali oleh enam turbin Rushton telah dilakukan untuk menyiasat kesan parameter yang berkesan untuk proses pencampuran. Kajian ini bertujuan untuk menilai parameter berpotensi yang mempengaruhi proses pengoptimuman dan memberikan gambaran terperinci ke dalam proses. Aliran tiga dimensi dan mantap telah dilakukan menggunakan teknik Rangka Rujukan Seragam (MRF) yang penuh ramalan untuk geometri pendesak dan tangki. Pengoptimuman proses sentiasa digunakan untuk memastikan keadaan optimum dipenuhi untuk mencapai kepuasan atau keperluan industri (iaitu meningkatkan keuntungan, kos rendah, hasil, dan lain-lain). Dalam kajian ini, pelbagai kelajuan yang dicadangkan untuk mempercepatkan pengoptimuman masing-masing adalah 100, 150 dan 200rpm dan julat kelulusan yang dicadangkan masing-masing adalah 50, 75 dan 100mm untuk pendesak dual Rushton. Oleh itu, dinamik cecair komputer (CFD) diperkenalkan untuk menyaring parameter yang sesuai dengan cekap dan mempercepatkan pengoptimuman.*

**Keywords:** Mixing process, CFD, screen parameters

### INTRODUCTION

Mixing process is widely used in industries, which covers vast application such as homogenizing viscous complex liquids for polymer blending, paints and solution polymerization (Edward et al. 2004). Moreover, mechanically stirred vessels are widely used for mixing of single phase flow and blending of homogenous liquids such as lube oils, gasoline additives, dilution in the chemical, mineral processing, wastewater treatment and other industries

(Montante and Magelli 2004). In order to achieve the best quality of products and production costs, the mixing process efficiency and optimization are the main parameters to be tackled (Zadghaffari et al. 2010). Nevertheless, according to Montate and Magelli 2004, if the spacing between the impeller is decreased as small as diameter of tank/3, the region between the turbines will behave as anisotropic, the merging or diverging of flow. Thus, if the distant between impeller is very dominant, they will produce single impeller profilr to ensure no interaction between adjacent impellers.

Recently, the Computer Fluid Dynamics (CFD) techniques have been fully utilized to substitute the experiments by providing detail explanations of the flow field which are impossible for experiments to be conducted. In order to model the flow behavior, the Reynolds averaging turbulent Navier-Stokes (RANS) equations and modeling Reynolds stresses with appropriate turbulence model has been adopted (Jenne and Reuss 1999). Besides, to account for impeller revolutions simulations in CFD, the technique of sliding Mesh (SM) and Multiple Reference Frame (MRF) have been widely introduced (Jaworski et al. 2000, Jaworski & Dudczak 1998, Cao et al. 2009).

The Rushton turbine is chosen in this study since it is a well established impeller for many tasks especially mixing of liquids with low velocities and has good gas dispersion properties (Jenne and Reuss 1999, Vrabel et al. 2000). Therefore, the purpose of the study is to investigate and to screen the parameters using CFD approach which affect the mixing efficiency in order to accelerate optimization.

## METHODOLOGY

### *Stirred vessel configurations*

In this study, ANSYS 13 software was fully utilized to draw the geometry of the object and data processing respectively. The dual Rushton impeller on the common shaft was used throughout this study. The height of fluid volume was fixed at 350mm and there are inlet and outlet pipe as well. The diameter of vessel is 218mm and the diameter of impeller is 100mm. The standard Rushton turbine is having six pedals with 90° angles. Figure 1 shows the schematic diagram of the experimental rig of this study. Figure 2 shows the dimension of standard Rushton turbine in this study. The speed of impeller is fixed at 50,100,150, 200rpm and the height of clearance is 25, 50, 75, 100mm respectively.

### *Modelling and numerical aspects*

In the present work, single phase, steady-state CFD simulations were performed and the results were post-processed in order to determine the effect of aforementioned parameters (ie, mixing speed and clearance) to the mixing process. These simulations were conducted with the commercial package ANSYS 13 using the traditional k-ε turbulence model (Alexopoulos et al. 2002). The standard k-ε model was implemented as it is the most widely used two equation eddy viscosity model and also for modeling turbulence in stirred tank reactor (Jenne & Reuss 1999). For simulating the flows generated by the impeller, Multiple Reference Frame was adopted (Cao et al. 2009). The whole vessel was divided into two regions: the moving one and the tank volume. In this way, the the effects of the blade rotations were accounted by the reference frame. The convection term in the governing equation was modeled with the first-order scheme and SIMPLE algorithm was used to resolved the coupling between velocity and pressure (Cao Xiao-chang et al. 2009). The criterion of 10<sup>-3</sup> was set for the convergence of solution. In this study, the boundaries of inlet and outlet and also moving zone were assigned to mass flow rate, pressure outlet and continuum respectively.

### *CFD Simulation*

Tet/hybrid with type TGrid mesh was dominating tank domain for efficient mesh resolution and interval size of 8 and 5 were used for tank zone and moving zone respectively to accommodate the complex impeller geometry. There were about 236k computational cells for moving zone and 107k computational cells for the tank domain. Figure 3 shows the meshing grid of the mixing vessel using tethybrid/TGrid.

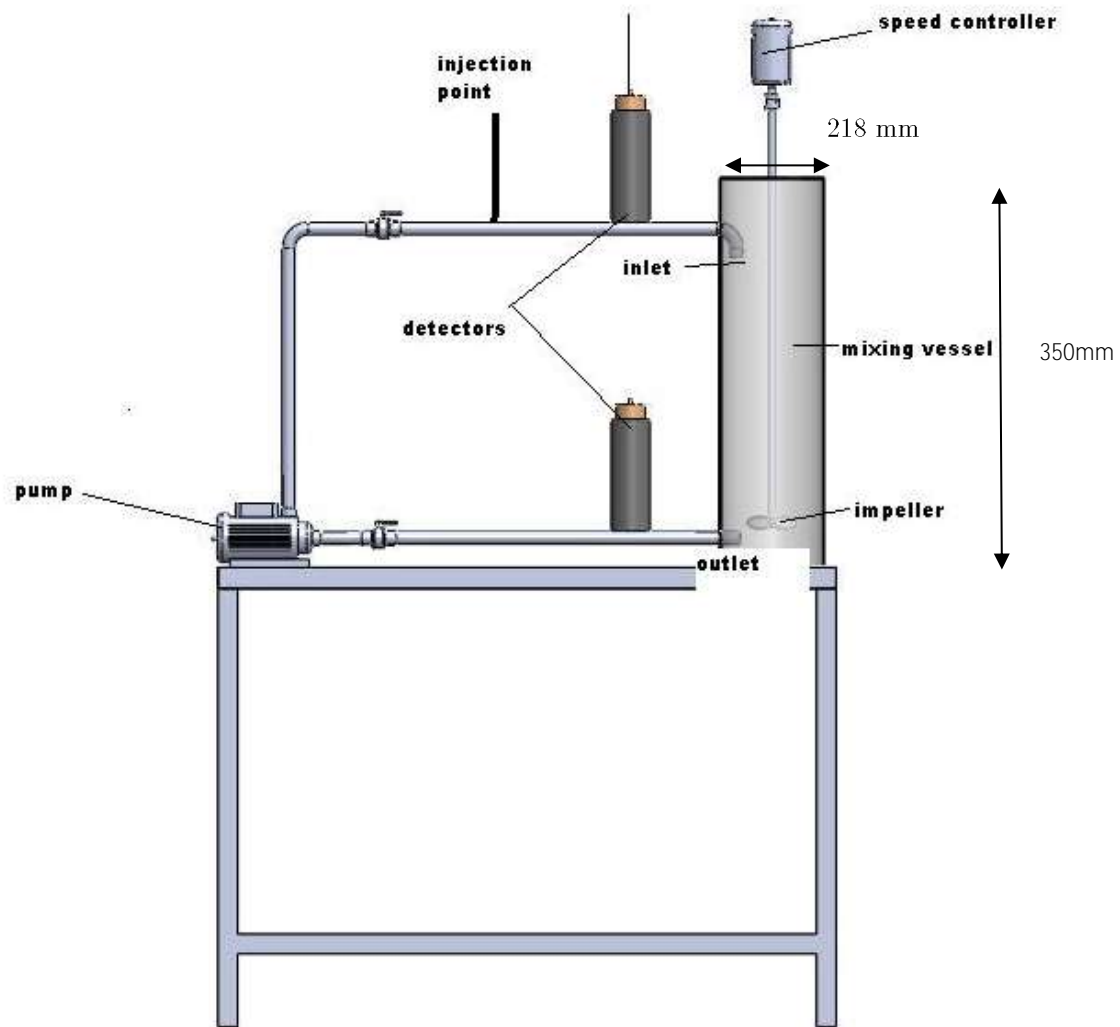


Figure 1. Diagram of mixing vessel rig for radiotracer experimentation

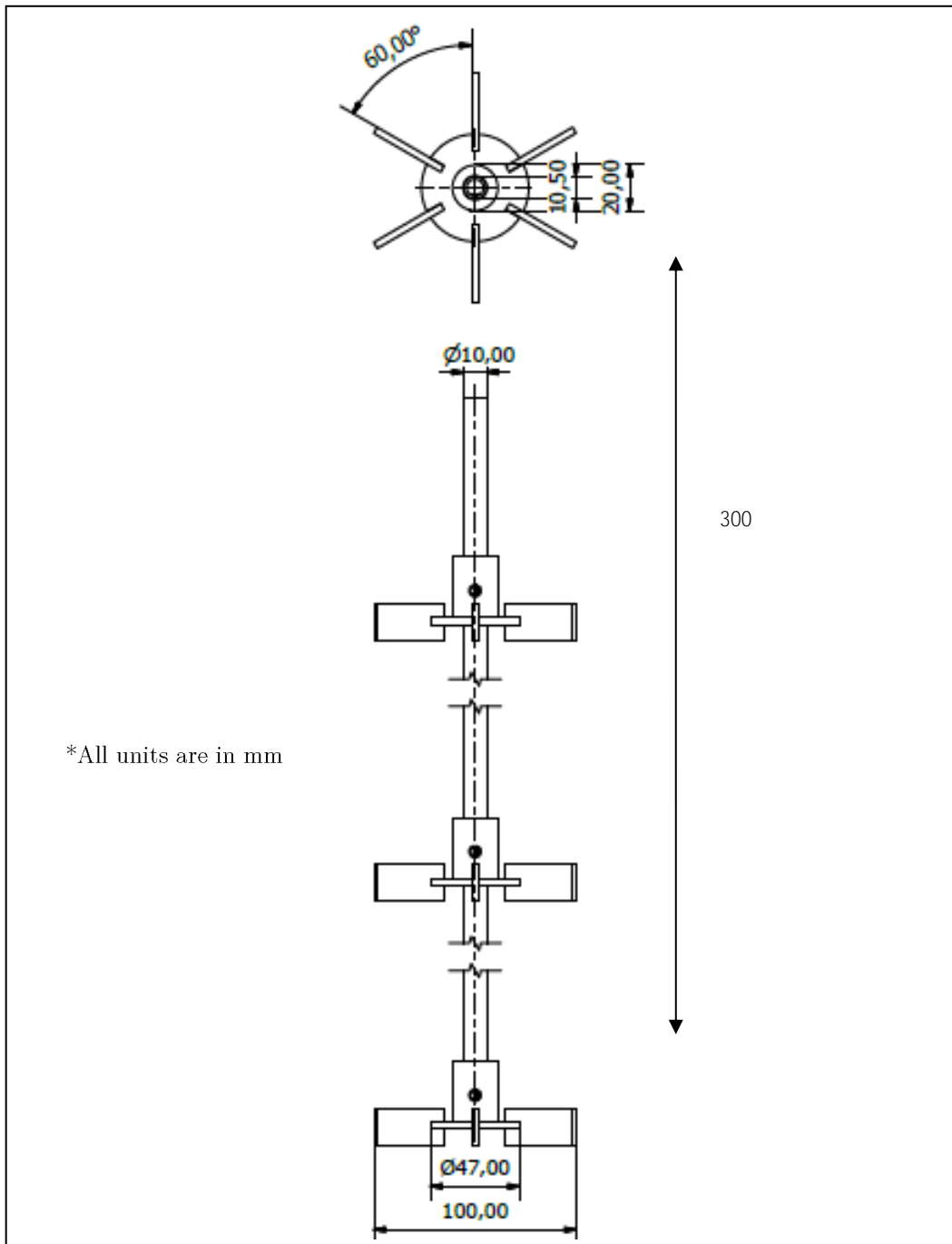


Figure 2. The dimension of standard Rushton turbine

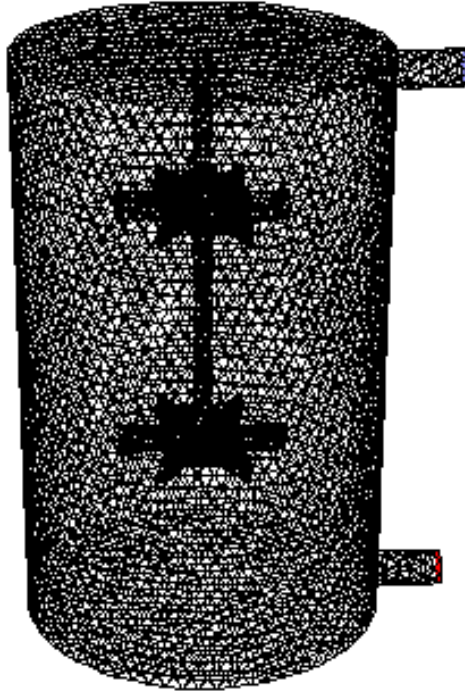


Figure 3. Meshing grid of the mixing vessel using tethybrid/TGrid.

## RESULTS AND DISCUSSIONS

### *Screening of parameters for Rushton turbine dual impellers: Qualitative analysis*

As a reference point, the iso-surface was created at x-axis in order to ensure all the captured images provide identical dimension. In this study, the rectangular dimension from Fluent was developed with dimension 530 mm x 900 mm. It can be observed from Figure 4 that the flow field exhibited a stronger circulation pattern extending over the large volume of the vessel. Nevertheless, at the top of the vessel near the shaft, the low velocity was identified and agreed by observations by Zadghaffari et al. 2010. Thus, from observations the speed of 50 rpm was eliminated to accelerate optimization since the dead volume was very imminent compared to others. In this study, the clearance of the bottom impeller from the bottom of the floor is 50 mm. Nevertheless, from the captions, it can be concluded that at clearance 50 mm, most of the liquid below the impeller was swept away. Thus, this clearance is selected as one of the set parameters. The dead zone is defined when the speed of liquid is 0.00 m/s and denoted as dark blue as in figures.

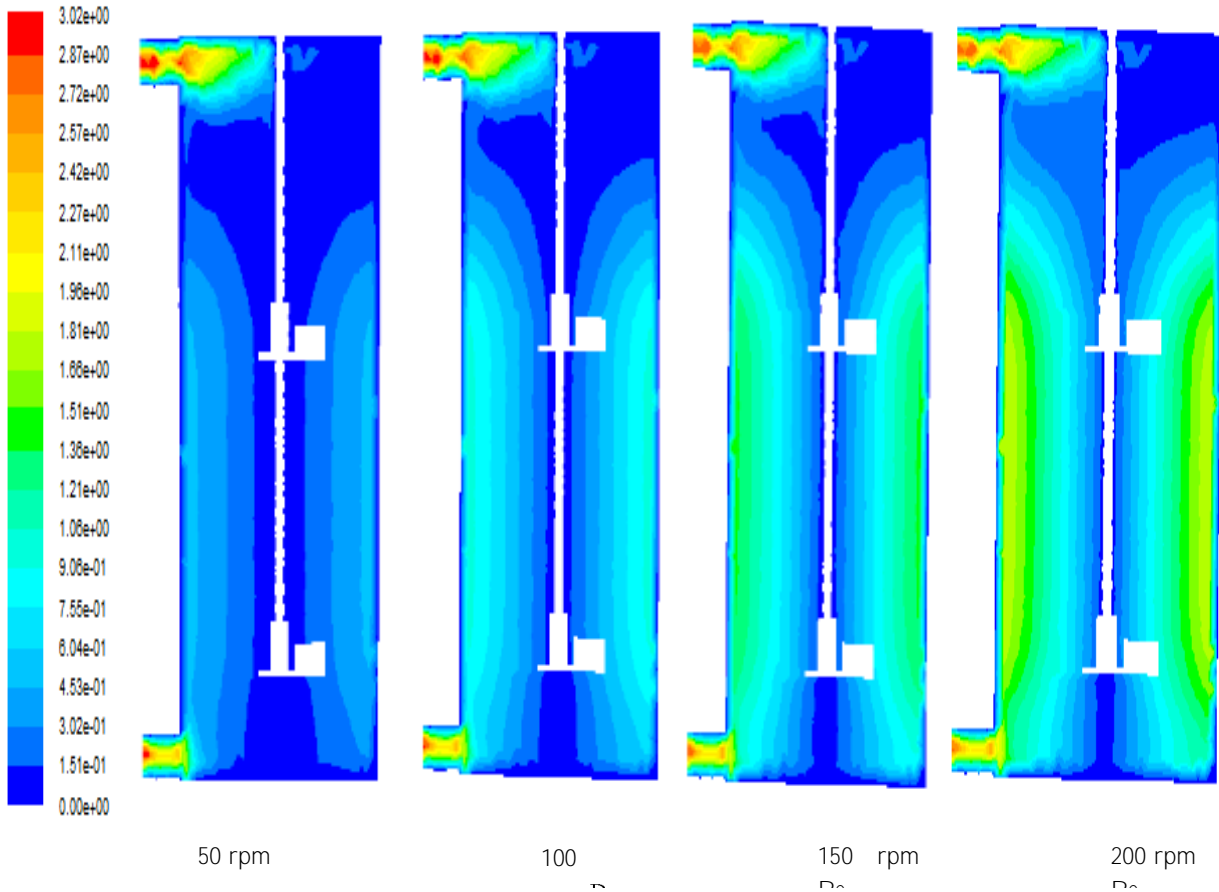


Figure 4. Velocity magnitude profile at 50mm clearance

In Figure 5 where the clearance was at 100 mm, similar results were obtained as Figure 5 in which the dead zone was found most when the speed of impeller was 50 rpm. Nevertheless in this stage, the dead zone contributions were coming not only from the top of impeller but from the bottom impeller as well. The increment of the dead zone coverage is due to the fact that the ability of the impeller to sweep the bottom floor when extended from 50 mm to 100 mm. According to Jenne and Reuss 1999, the flow field below the impeller has a positive tangential velocity component like the radial-tangential jet which originates from the impeller. The flow also tends to direct to the vessel wall.

Figure 6 shows velocity magnitude profile at 25 mm clearance. From observations, the dead zone was increasingly reduced at the bottom of impeller when the clearance was set at 25 mm for all range of speed. Nevertheless as the height of volume was set at 350 mm, the percentage of dead zone was increased tremendously on the top of impeller. Thus, the clearance of 25mm was removed from the option of optimization. Perhaps, the best way to tackle the issue is to add another impeller in between to make up to three instead of two impellers. Nevertheless, in this study it is not possible to put another impeller since the mixing involves radiation material in which the tendency of the splashing of radioactive mixture is possible.

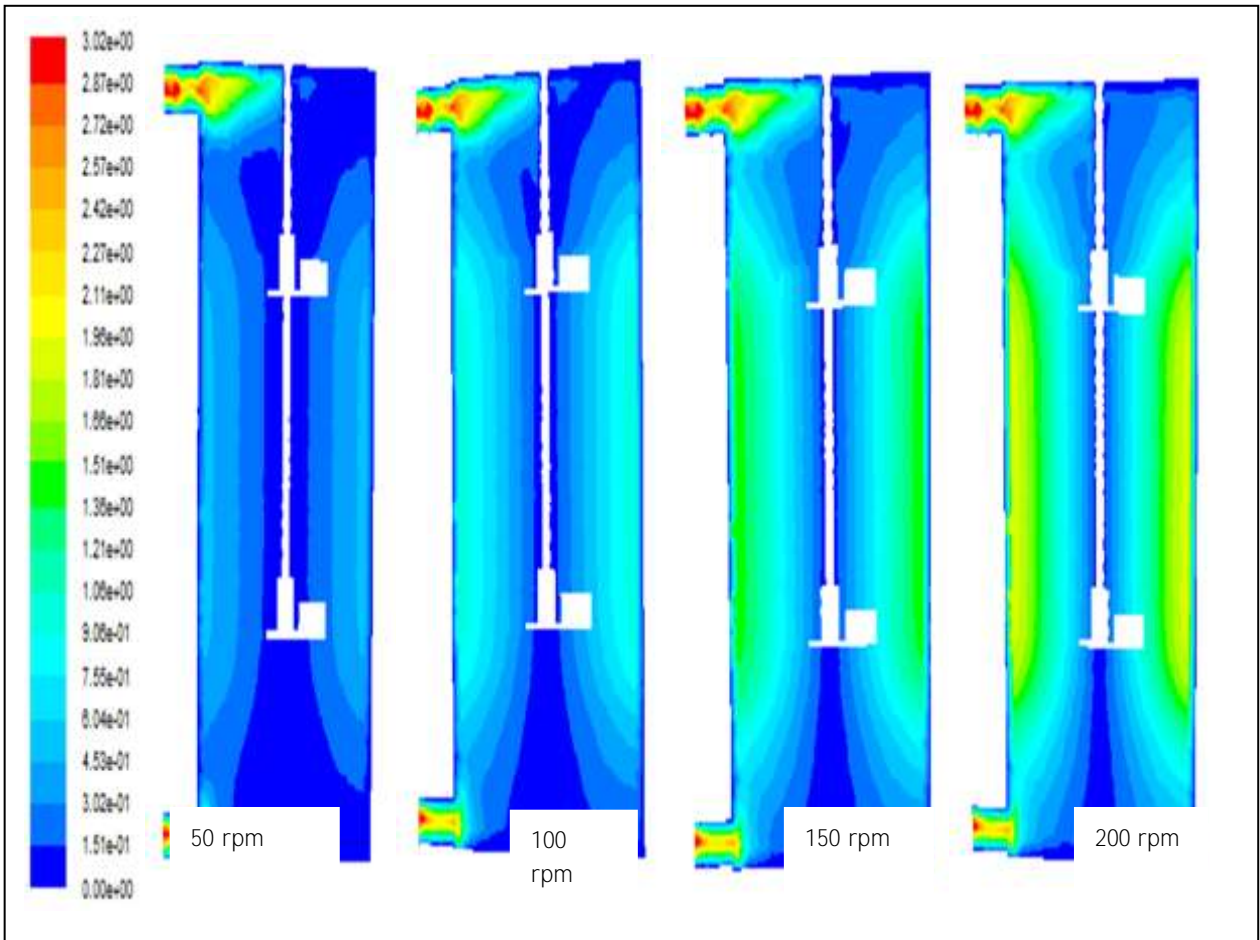


Figure 5. Velocity magnitude flow profile at 100 mm clearance

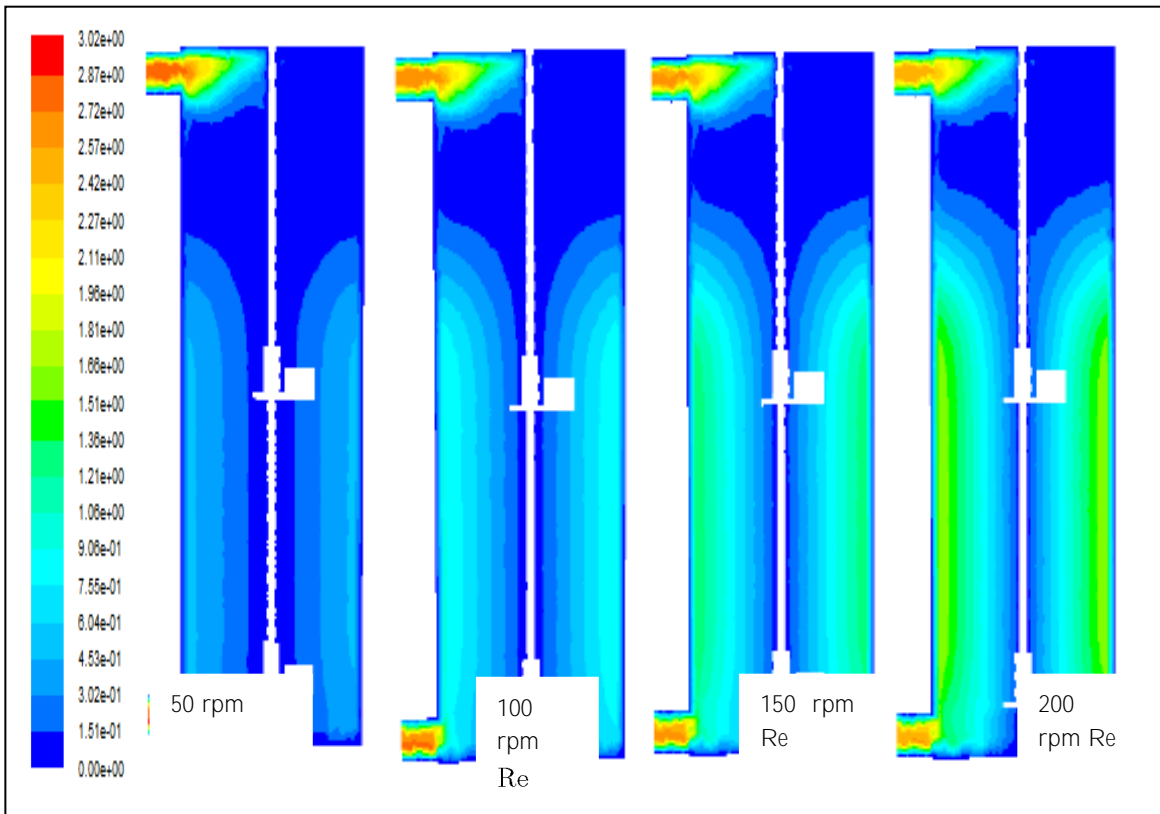


Figure 6. Velocity magnitude profile at 25mm clearance

Figure 7 shows velocity magnitude profiles at 75 mm clearance. It shows that all range of speeds were able to homogeneously mix the liquid except for the speed of 50 rpm. The dead zone was subsequently reduced as we increased the speed and the presence of dead zone was almost balance at the top and bottom of impeller. Thus, in this study, the range of recommended speed to accelerate optimization is 100, 150 and 200rpm respectively and the range of recommended clearance is 50, 75 and 100 mm respectively for dual Rushton impeller. Overall, the increment of clearance from 25 mm to 100 mm resulted in the formation of merging flow or double loop configuration (Montate and Magelli 2004) when the ratio of clearance to diameter ( $C/T$ ) of vessel increased from 0.11 to 0.46. Nevertheless, the results contradicted from Montate and Magelli 2004 whereby as  $C/T$  increased from 0.17 to 0.51, the flow changed from merging flow to parallel flow. Nevertheless, the contradiction might be due to the impeller speed used in their study was higher 860-900 rpm and there was no inflow and outflow in their studies. Moreover, according to the global flow pattern, two circulation liquid loops, which appear on the top and bottom of impeller, will be produced by one impeller (Vrabel et al. 2000).

#### Screening of parameters for Rushton turbine dual impellers: Quantitative analysis

From figure 8, we found that as the speed of impeller was increased, the percentage of dead zone decreased. It can be observed that as speed of impeller increased from 50 rpm to 200 rpm, the percentage of dead zone was tremendously reduced by as high as 73.59% to 11.77% respectively. It is because as the rpm increases, the Reynolds number is increased. Thus, the stronger radial out flow pushes the species rapidly into the lower and upper recirculation loops, which reduces the mixing time as well as the dead zone (Zadghaffari et al. 2010). Nevertheless, the figure indicates that the high of clearance of dual Rushton turbine gives small effect to the removal of dead zone.



Dual Rushton impeller, clearance = 75mm

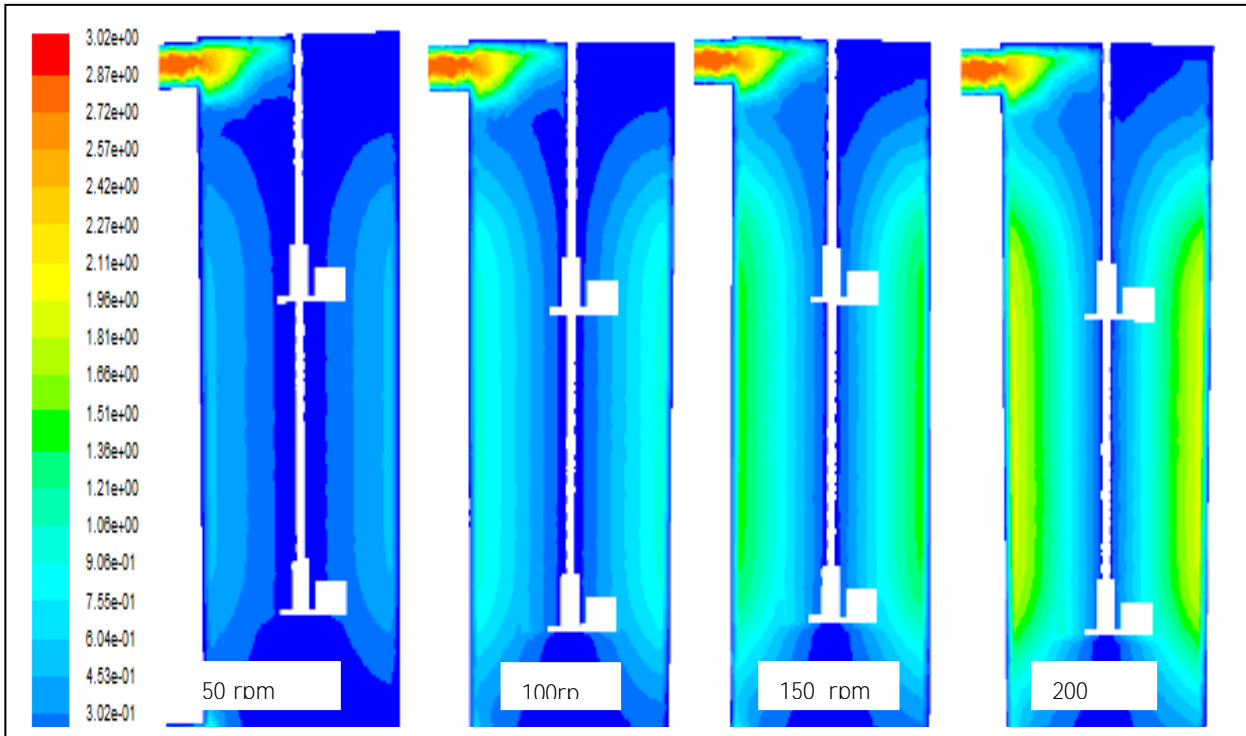


Figure 7. Velocity magnitude profile at 75mm clearance

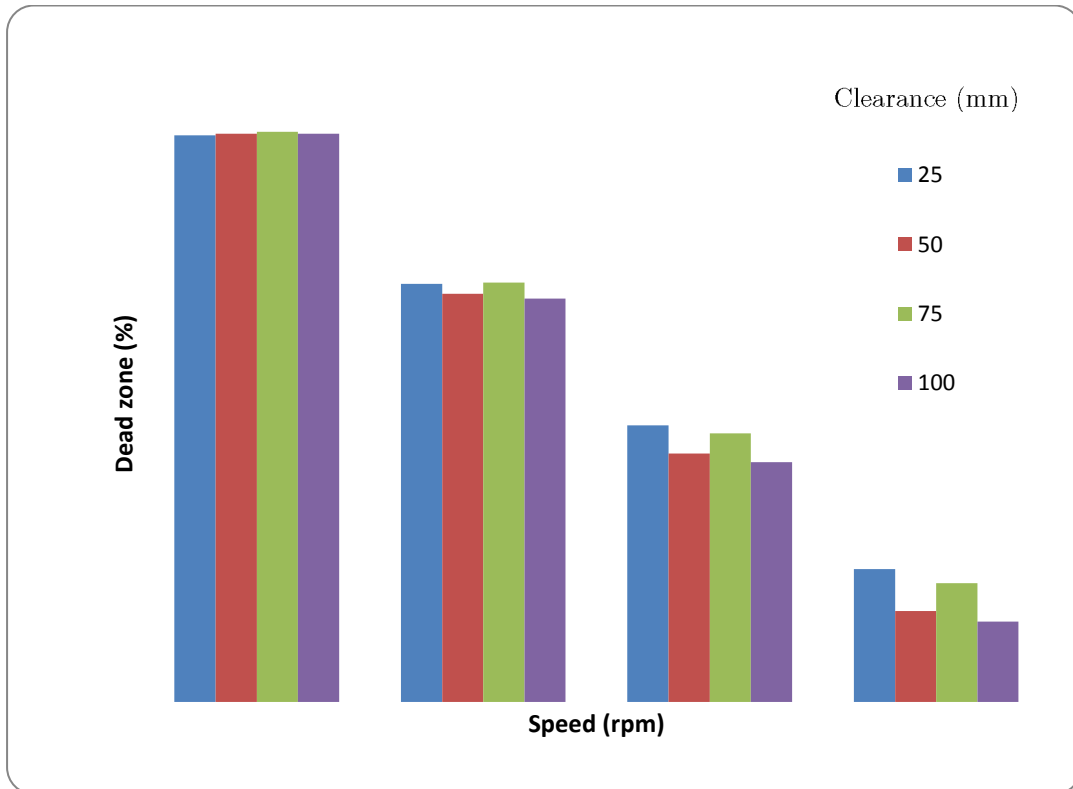


Figure 8. Percentage of dead zone with respect to speed of impeller

Figure 9 and 10 also show that dual impeller Rushton turbine contributes to the formation of axial and radial velocity. It can be observed from Figure 10 that there was descending trend of axial velocity percentage as the clearance height increased with respect to increasing of impeller speed. As the speed of impeller is increasing, the percentage of axial velocity was decreasing tremendously as well as the percentage of radial velocity although

the change was very minimum inter clearance height. According to Zadghaffari et al. (2010), the presence of imminent axial profile indicates that the impeller stream flows away from impeller blade which contributes to the variation of velocity in the axial direction. Thus, as the fluid moves away from the impeller, the impeller stream becomes flatter.

As can be observed also, the radial velocity was higher when clearance was 75mm. This is because the Rushton turbine generates radial and tangential flows which divide at the vessel wall and the flow then recirculates back into the impeller region. Recirculation of flow is the main reason for the mixing capability of stirred tank (Jenne and Reuss 1999). Thus, at clearance 75 mm, sufficient space is provided for the radial-tangential flow to occur in the vessel.

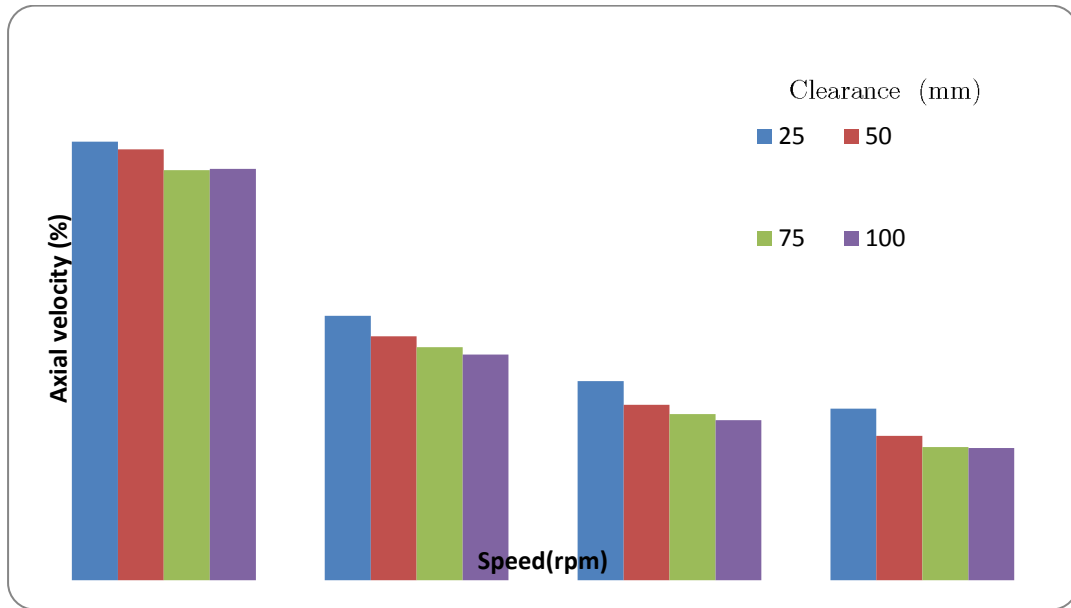


Figure 9. Axial velocity

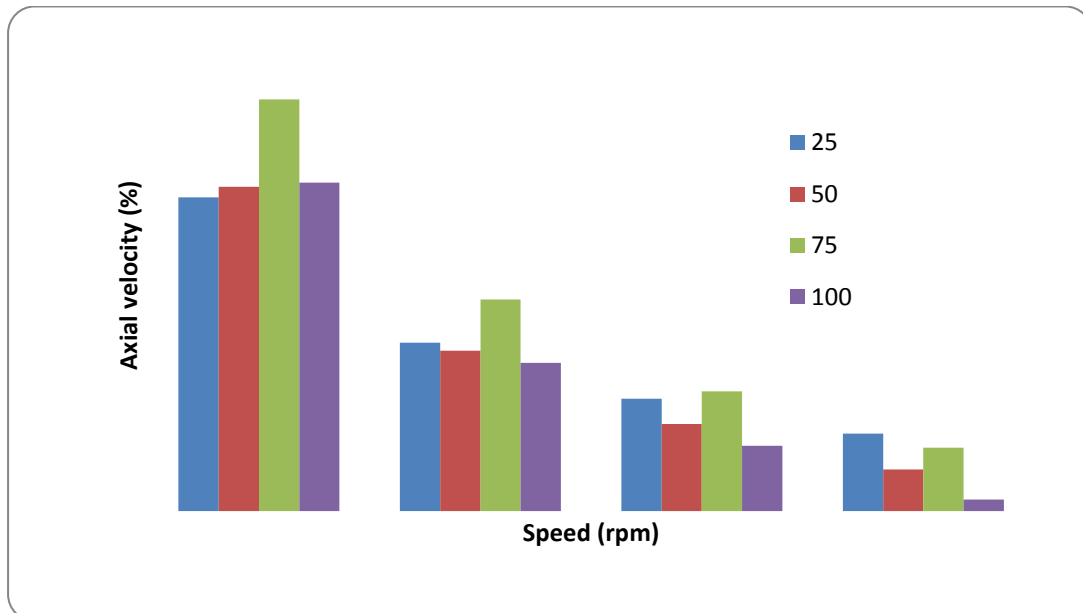


Figure 10. Radial velocity

**Validation**

Table 1 shows the comparison of findings from previous authors with regard to the mixing vessel studies.

Table1

Geometrical parameters for multi impellers (mm)

	This study (2012)	Zadghaffari et al. 2009	Jaworski et al. 2000
No. of impeller	2	2	2
Type of impeller	Rushton	Rushton	Rushton
Tank diameter (T) (mm)	218	300	720
Depth of liquid (H)	1.6T	1.8T	2T
Impeller diameter (D)	100	T/3	T/2
Impeller blade width (w)	3	nil	nil
Impeller blade height (h)	16	nil	nil
Baffle width (B)	nil	T/10	nil
Impeller clearance (C)	0.68T	0.55T	T/4
Speed (rpm)	50,100, 150	200, 250	75, 100, 150

CONCLUSIONS

In this study, the range of recommended speed to accelerate optimization is 100, 150 and 200rpm respectively and the range of recommended clearance is 50, 75 and 100mm respectively for dual Rushton impeller. It can be concluded that numerical simulation has successfully assisted in screening the effective parameters for mixing efficiency in this study.

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