CFD study of mixing miscible liquid with high viscosity difference in a stirred tank

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Abstract. The mixing process of miscible liquids with high viscosity difference is crucial role even though the solution mutually dissolved. This paper describes the mixing behaviour of the water-molasses system in a conical-bottomed cylindrical stirred tank (D = 0.28 m and H = 0.395 m) equipped with a side-entry Marine propeller (d = 0.036 m) under the turbulence regime using a three-dimensional and transient CFD-simulation. The objective of this work is to compare the solution strategies was applied in the computational analysis to capture the detail phenomena of mixing two miscible liquid with high viscosity difference. Four solution strategies that have been used are the RANS Standards k-ε (SKE) model as the turbulence model coupled with the Multiple Reference Frame (MRF) method for impeller motion, the RANS Realizable k-ε (RKE) combine with the MRF, the Large Eddy Simulation (LES) coupled with the Sliding Mesh (SM) method and the LES-MRF combination. The transient calculations were conducted with Ansys Fluent 17.1 version. The mixing behaviour and the propeller characteristic are to be compared and discussed in this work. The simulation results show the differences of flow pattern and the molasses distribution profile for every solution strategy. The variation of the flow pattern which happened in each solution strategy showing an instability of the mixing process in stirred tank. The LES-SM strategy shows the realistic direction of flow than another solution strategies.

1.  Introduction

Based on the type of fluid, the categories of the multiphase flow divided into gas-liquid, solid-liquid and liquid-liquid. The liquid-liquid mixing divided into immiscible liquids dispersion and miscible liquids blending, the latter of which is the primary focus of the present work. The mixing process of miscible liquids is crucial role even though the solution mutually dissolved. Homogenization of miscible liquids achieves slowly by molecular diffusion and natural convection, but agitated can obtain homogenous condition more quickly. The application of mixing of miscible liquids is in bioethanol industrial which uses molasses as the raw material.

Advances in computer technology and mathematical model have enabled researchers to conduct the fluid dynamic investigation computationally. The computationally study of mixing process more efficient than experimentally. The Computational Fluid Dynamics (CFD) has become a powerful the tools to conduct the fluid dynamic investigation, and it has been successfully used to predict the...
mixing behaviour inside stirred tank. The CFD study on mixing inside stirred tank mostly evaluating the top-entry impellers configuration. Little work has done on studying the side-entry impellers configuration by CFD method, i.e. the homogenization of crude oil [1], the effect of propeller layout on mixing time of crude oil [2], the effect of impeller layout on mixing intensity on the solid-liquid system [3] and the mixing of pseudoplastic solutions [4].

So far, the study on the computational fluid dynamic about the mixing of the miscible liquids inside stirred tank is limited, among others, the blending of ethanol and glycerol with an anchor impeller [5] and the homogenization of two miscible liquid with a pitch blade turbine [6]. The water-molasses process of mixing in a stirred tank under turbulence regime is subject of our research; the previous work has done to compare the mixing behaviour of top-entry impeller configuration and side-entry impeller configuration [7]. The specific concern on the appropriate solution strategy which was applied to determine the mixing behaviour inside the tank is the subject of this present paper. The main differences include the use of different modelling turbulence and impeller motion model.

Fluid flows inside stirred tank mostly under the turbulence regime, selection of turbulence models is crucial to obtain a velocity flow fields. The Direct Numerical Simulations (DNS), the Large Eddy Simulation (LES) and the Reynolds-Averages Navier-Stokes (RANS) were included in the turbulence approach. The DNS resolves all turbulent length and time scales by directly integrating the Navier-Stokes equation while in LES, large eddies are resolved directly, and small eddies are modelled [8]. On the other hand, the Reynolds-averaged Navier-Stokes (RANS) equations amount to averaging out the large eddies. The RANS model involved the Standard k-ε (SKE) model [9], the Renormalization k-ε (RNG) model [10] and the Realizable k-ε (RKE) model [11]. The RNG k-ε model more accurate and reliable for a wider class of flow than the SKE model, however, the RKE model provides the best performance [12].

The Sliding Mesh (SM) method and the Multiple Reference Frame (MRF) method was applied to determine the impeller motion. The SM method is a fully transient approach where the rotating mesh slides relatively to the stationary mesh, and no needs experimental boundary condition because the flow around the impeller blades is being calculated in detail [13]. The MFR is a steady flow field in which predicted the relative motion between the rotating frame and stationary reference frame. In MRF model, impeller region is modelled as stationary, and tank wall is modelled as rotating zones [14].

Another important factor that can not be ignored in stirred tank study is to characterise the impeller; the power number is one. Power number (N_p) is the amount of energy required per unit time in a mechanical agitation in stirred tank [15]. Power consumption (P) is the power delivered to the fluid (the product of the impeller speed, 2πN, in rad/s) and measurement of torque (T_q) :

\[ P = 2\pi N T_q \]  

The power number (N_p) can be calculated by:

\[ N_p = \frac{P}{\rho N^3 D^5} \]  

The objective of this work is to compare the solution strategies which was applied in the computational analysis on mixing of two miscible liquid with high viscosity difference inside conical-bottomed cylindrical stirred tank equipped with a side-entry Marine propeller using the CFD method to capture the mixing behaviour and propeller characteristic.

2. Computational fluid dynamics methods

In this present work, the model equations numerically solved by adopting the finite volume. The three-dimensional and transient CFD-simulation was conducted with Ansys Fluent 17.1 version under the turbulence regime. The simulation is divided into four solution strategies, i.e. SKE-MRF, RKE-MRF, LES-SM and LES-MRF. The parallel calculation was performed using HP Z620 workstation with 12 cores and Windows 8 64 bit operating system.
2.1. Geometry system  
The geometry system is a conical-bottomed cylindrical stirred tank with a diameter of 0.28 m and height 0.395 m. The geometry generated using Ansys Design Modeller software. The tank is equipped with a three-blade Marine propeller (d = 0.036 m) as can be seen in Figure 1, installed with side-entry configuration.

![Figure 1. The geometry of Marine propeller and moving zone](image1)

![Figure 2. The stirred tank geometry](image2)

![Figure 3. The observation plane](image3)

The propeller mounted on the conical side of the tank with angle of 45° and located at a distance of 0.044 m from the bottom of the tank as shown in Figure 2. The flow domain is discretized through grids (122,468 nodes) by Ansys Meshing software and evaluate the quality of meshing using skewness methods. The result of simulation was analysed through the observation plane as shown in Figure 3.
2.2. Fluid flow approach and solution setup
The solver is pressure-based, and the gravitational acceleration is active at y-axis was set to -9.81 m/s². All the simulation was applied a Mixture model multiphase flow [12] under a turbulence regime with propeller rotational speed (N) set at 1000 rpm and time step 0,01 s. For the first solution strategy (SKE-MRF) is using the RANS (SKE) as the turbulence model [16] coupled with MRF as the rotational impeller method while the second solution strategy (RKE-MRF) is a combination of RANS (RKE) [11] with MRF. Moreover, the third solution strategy (LES-SM) was applied the Large Eddy Simulation (LES) approach with the WMLES S-Omega subgrid-scale turbulence model [17] coupled with the fully transient Sliding Mesh (SM) methods for simulating the propeller motion. The fourth solution strategy is using LES combined with MRF method. The solutions methods applied for every solution strategy as can be seen in Table 1.

2.3. Boundary condition
The fluid used are molasses (μ = 2.09 Pa.s) and water (μ = 0.001003 Pa.s). To define the initial condition, the height of molasses inside the tank is set at 0.158 m, and the height of water fills the tank is set at 0.235 above molasses. To define the boundary condition, the flow domain is divided into two parts, i.e. moving zone and static zone. The interfaces between moving zone and static zone treated as interface boundary condition. The shaft regarded as an absolute moving wall and the propeller is a moving wall in which relative to moving zone. The tank wall is a stationary wall and treated as the no-slip condition. The boundary condition at the liquid surface was set to symmetry because the shear stresses are zero.

| Solutions Methods         | SKE-MRF                           | RKE-MRF                           | LES-SM                           | LES-MRF                           |
|---------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|
| Pressure – Velocity coupling | Semi-Implicit Method for Pressure-Linked Equation (SIMPLE)[18] | The Pressure-Implicit with Splitting of Operator (PISO)[19] | Least Squares Cell-Based*         |                                    |
| Gradient                  |                                    |                                   |                                   | Pressure Staggering Option (PRESTO)[20] |
| Pressure                  |                                    |                                   |                                   | Bounded Central Differencing [21]  |
| Momentum                  |                                    |                                   |                                   | First Order Upwind*               |
| Volume fraction           |                                    |                                   |                                   | First Order Upwind*               |
| Turbulent kinetic energy  |                                    |                                   |                                   |                                    |
| Turbulent dissipation rate|                                    |                                   |                                   |                                    |
| Transient formulation     |                                    |                                   |                                   |                                    |

* [12]

3. Result and discussion
The mixing behaviour of two miscible liquid with high viscosity difference inside stirred tank is reviewed based on the flow pattern which is represented by the vector analysis of the flow velocity and the molasses distribution profile indicated by the density contour and prediction value of density mixture. Analysis of power number also carried out to show the propeller characteristic.
3.1. Flow pattern and molasses distribution profile

Based on Figure 4, it appears that the Marine propeller generates flow pattern with an axial direction and forms loop circulation of the fluid flow. However, there is a difference in the direction of the flow. Fluid flow with SKE-MRF solution strategy at 340 s which shown in Figure 4(a) indicates that the fluid is sucked and flow out towards the negative axial direction to the bottom of the tank towards the impeller, then it deviates changing its direction pushed upward towards the positive axial direction. Then the fluid flows radially to the negative axial direction towards the bottom of the tank and forms a double loop circulation inside the tank.

![Flow pattern generated by Marine propeller for different solution strategy: (a) SKE-MRF; (b) RKE-MRF; (c) LES-SM; and (d) LES-MRF](image)

**Figure 4.** Flow pattern generated by Marine propeller for different solution strategy: (a) SKE-MRF; (b) RKE-MRF; (c) LES-SM; and (d) LES-MRF

The phenomenon of mixing generated by the SKE-MRF solution strategy is similar to the phenomenon of mixing produced by the RKE-MRF and the LES-MR solution strategy as shown Figure 4(b) and Figure 4(d), respectively. The loop circulation causes the mixing process of molasses and water which occurs in the tank as seen in Figure 5(a),(b) and (d). When the mixing process begins, water is sucked into the molasses-rich area at the bottom of the tank. It causes the molasses
concentration reduced. Then the water slowly diffused with molasses and formed some layer at the interface section. The contour analysis resulting from the LES-MRF solution strategy as seen in Figure 5(d) indicated a more quickly reach the homogenous condition than the two previous solution strategies (SKE-MRF and RKE-MRF).

![Density Contour](image)

**Figure 5.** Density contour at 340 s for different solution strategy: (a) SKE-MRF; (b) RKE-MRF; (c) LES-SM; and (d) LES-MRF

Based on Figure 4(e), it can be seen that the direction of the flow is moving to the bottom of the tank towards the negative axial direction then deviates towards the impeller. The fluid is pumped out towards the negative axial direction then forms loop circulation around the tank. There are some unstable flows and loops which are formed along the tank wall. The significant different in the
direction of flow and flow pattern happened when using the Sliding Mesh impeller motion model. The motion of the impeller generated by the Sliding Mesh method shows the realistic direction of flow.

The Sliding Mesh method is suitable for the prediction of flow pattern in stirred tank [22]. Other than that, based on Figure 5(c) the density contour produced by LES-SM solution strategy shows the significant changes in the molasses distribution than another solution strategies.

The CFD simulation generates the prediction value of the density mixture as a function of time as shown in Figure 6. It indicates that the density changes yielded by LES-SM solution strategy show the significant decrease and it reveals that the homogeneous condition reached sooner than the other solution strategies.

![Figure 6](image)

**Figure 6.** The density changes inside stirred tank as a function of time for different solution strategy

3.2. Propeller characteristic

The power number analysis represents the propeller characteristic in this work. The analysis of the power number generated by the propeller for all solution strategies is shown in Figure 7. Based on that graph, the power number prediction value generated by the LES-SM solution strategy is significantly different from three other solution strategies. The power number prediction value as a result of the LES-SM solution strategy is in accordance with the literature [23].

![Figure 7](image)

**Figure 7.** The power number produced by Marine Propeller for various solution strategies as a function of time
Furthermore, the graph trend on LES-SM solution strategy denotes that as the time goes by the value of power number decrease while the other solution strategies tend to indicate a constant trend. It represents that the power required for mixing process is reduced as the length of mixing time and the homogeneity of the mixture is increased.

4. Conclusion
In the presents work, the mixing of two miscible liquid with high viscosity difference inside conical-bottomed cylindrical stirred tank equipped with the side-entry Marine propeller in four different solution strategies (SKE-MRF, RKE-MRF, LES-SM and LES-MRF) at 1000 rpm was investigated via three-dimensional and transient CFD-simulation. The CFD-simulation result shows the mixing behaviour inside the stirred tank and the propeller characteristic for every solution strategy. The variation of the flow pattern which happened in each solution strategy showing an instability of the mixing process in stirred tank. The CFD analysis led to conclude that the flow direction generated by propeller as a result of the LES-SM solution strategy shows more realistic than another solution strategies. The prediction value of power number ($N_p$) generated by the LS-SM solution strategy is in accordance with the literature. Moreover, on the LES-SM solution strategy, signify that the density changes more quickly to reach the homogeneous condition than another solution strategies. The Sliding Mesh impeller motion approach generates the significant effect on the propeller characteristic and flows direction; this influences the molasses distribution inside the stirred tank. Further validation of these models by visual experimental and grid dependent test to determine the minimum grid is necessary will have to perform.

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References
[1] Dakhe A A and Rahimi M 2004 CFD simulation of homogenization in large-scale crude oil storage tanks Journal of Petroleum Science and Engineering 43(3–4) pp 151-161
[2] Rahimi M 2005 The effect of impellers layout on mixing time in a large-scale crude oil storage tank. Journal of Petroleum Science and Engineering 46(3) pp 161-170
[3] Wu B 2011 CFD investigation of turbulence models for mechanical agitation of non-Newtonian fluids in anaerobic digesters Water Research 45(5) pp 2082-2094
[4] Sossa-Echeverria J and Taghipour F 2015 Computational simulation of mixing flow of shear thinning non-Newtonian fluids with various impellers in a stirred tank Chemical Engineering and Processing: Process Intensification 93 pp 66-78
[5] Al-Qaessi F and Abu-Farah L 2009 Prediction of mixing time for miscible liquids by CFD simulation in semi-batch and batch reactors Engineering Applications of Computational Fluid Mechanics 3(1) pp 135-146
[6] Derksen J J 2011 Blending of miscible liquids with different densities starting from a stratified state Computers & Fluids 50(1) pp 35-45
[7] Madhania S et al 2017 Mixing behaviour of miscible liquid-liquid multiphase flow in stirred tank with different marine propeller installment by computational fluid dynamics method Chemical Engineering Transactions 56 pp 1057-1062
[8] Bakker A and Oshino L M 2004 Modelling of turbulence in stirred vessels using large Eddy simulation Chemical Engineering Research and Design 82(9) pp 1169-1178
[9] Launder B E and Spalding D B 1974 The numerical computation of turbulent flows Computer Methods in Applied Mechanics and Engineering 3(2) pp 269-289
[10] Yakhot V and Orszag S A 1986 Renormalization group analysis of turbulence. I. Basic theory Journal of Scientific Computing 1(1) pp 3-51
[11] Shih T H et al 1995 A new k-ε eddy viscosity model for high reynolds number turbulent flows Computers & Fluids 24(3) pp 227-238
[12] ANSYS-Fluent 2016 Fluent 17.1 Documentation Fluent Theory Guide Lebanon, N.H., USA: ANSYS Inc
[13] Marshall E M and Bakker A 2004 Computational fluid mixing, in handbook of industrial mixing John Wiley & Sons Inc. pp 257-343
[14] Luo J Y , Issa R I and Gosman A D 1994 Prediction of impeller induced flows in mixing vessels using multiple frames of reference, in I. Chem. E. Symposium series 136. 1994 Cambridge UK pp 549-556
[15] Zadghaffari R, Moghaddas J S and Revstedt J A 2009 mixing study in a double-Rushton stirred tank Computers & Chemical Engineering 33(7) pp 1240-1246
[16] Yang C and Mao Z S 2014 Chapter 3 - Multiphase stirred reactors, in Numerical Simulation of Multiphase Reactors with Continuous Liquid Phase Academic Press: Oxford pp 75-151
[17] Shur M L et al 2008 A hybrid RANS-LES approach with delayed-DES and wall-modelled LES capability. International Journal of Heat and Fluid Flow 29(6) pp 1638-1649
[18] Van Doormaal JP and Raithby G D 1984 Enhancements of the simple method for predicting incompressible fluid flows Numerical Heat Transfer 7(2) pp 147-163
[19] Issa R I 1986 Solution of the implicitly discretised fluid flow equations by operator-splitting J. Comput. Phys. 62(1) pp 40-65
[20] Bender E 1980 Numerical heat transfer and fluid flow. Von S. V. Patankar. Hemisphere Publishing Corporation, Washington – New York – London. McGraw Hill Book Company, New York 1. Aufl., 197 S., 76 Abb., geb., DM 71,90. Chemie Ingenieur Technik 53(3) pp 225-225
[21] Leonard B P 1991 The Ultimate conservative difference scheme applied to unsteady one-dimensional advection Computer Methods in Applied Mechanics and Engineering 88(1) pp 17-74
[22] Bakker A et al 1997 Sliding mesh simulation of laminar flow in stirred reactors Chemical Engineering Research and Design 75(1) pp 42-44
[23] Hemrajani R R and Tatterson G B 2004 Mechanically stirred vessels, in handbook of industrial mixing John Wiley & Sons Inc. pp 345-390