CFD Simulation of Gas-Liquid in an Agitated Vessel

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Abstract

Background/Objectives: In chemical industries, understanding of fluid mixing is significant. The objective is to determine optimum conditions of gas-liquid mixing by changing impeller blade's gradient, number of impeller and rotation rate. **Methods/Statistical analysis**: In this work, by using a computational fluid dynamic (CFD); Ansys© Fluent software, we simulated numerically a gas-liquid mixing in an agitated vessel equipped with a pitched-blade impeller. In this study, the range of the impeller blade's gradient is between 0° to 90° with three number of impellers; impeller (a), (b) and (c) and the impeller rotation speed rate which is between 90 to 120 rpm are used. **Findings:** The reconstruction images of the nitrogen gas in the distilled water mixing in the agitated vessel are obtained from the Ansys© simulation. Based on the simulation results, the gradient of blades impeller at 60°, three numbers of impeller (c) and 90 rpm rotation rate are chosen as the optimum condition for well mixing condition for gas nitrogen in the agitated vessel. **Application/Improvements:** This modelling have various applications in optimization and design of a wide range of gas-liquid processes industry where the mixing process will affects about 25% of all process industry operations.

Keywords: Agitated Vessel, Ansys©, CFD, Gas-Liquid, Mixing, Pitched-blade Impeller

1. Introduction

Numerous major industrial operations such as oxidation, hydrogenation and biological fermentations involve in mixing of gases and liquids. This purpose of the mixing processes to agitate the mixture of gas-liquid to generate a gas bubbles' dispersion in a liquid phase. Generally, mixing affects around 25% of all process industry operations¹. The primary aim of mixing is to improve the interfacial mass transfer rate in the vessels, which is related to the interfacial area between phases, volume fraction hold-up, bubble or droplet or particle size distribution. Besides that, the aim of mixing is to achieve the dynamic equilibrium between coalescence and breakage rate, turbulence level, fluid properties of dispersed and continuous phases, and mechanical mixing parameters such as impeller size and model, vessel size, and flow velocity².

Various measurement techniques are established in order to determine the well-mixing process in the industry. For example, to determine the fluid's velocity and

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pattern in such vessel, the effect of stirrer blade gradient on the efficiency of gas-liquid mixing in the agitated vessel by using the Particle Image Velocity (PIV) technique³. It shows that the fluid flow velocity increases with increasing of pitched-blade impeller gradient⁴ studied shows that the pitched-blade impeller increase with the residence time in the gas-liquid mixing vessel guided by a mechanical motor. The work focused on four types of impeller blades i.e. impellers disk Rushton, impeller disc blade half circle, 45° pitched-blade impeller flow down and above. In addition, the Continuous Stirred Tank Reaction (CSTR) is designed for the polymerization methyl methacrylate process which equipped with six of 45° blade impeller⁵.

As it is impossible to determine and cover all the gas-liquid mixing process parameters experimentally, Computational Fluid Dynamics (CFD) has created opportunities to visualize the mixing phenomena⁶. CFD is able to predict fluid flows, chemical reaction rates, mass and heat transfer rates, and other occurrences by solving a set of appropriate mathematical equations⁷. In addition,

CFD also provides useful information for regions with intense or mild turbulence zones, Reynolds stresses, vortex structures, circulation patterns, flow behavior, and many other parameters⁶. Gradually, the CFD method is becoming a beneficial tool to study the complex fluid flow in the agitated vessels. Numerous of papers published⁸⁻¹⁰ discussed simulation methods for agitated vessel. Yet in the aforementioned literature, most simulations studied and focused only on the single-phase liquid flow, although often industries' applications include with gasliquid or solid-liquid mixtures. Therefore, comprehensive simulation techniques must be involved with contacting of multiphase flows.

Lots of simulations are studied and reported in the gas-liquid dispersion in the agitated vessels, and while the success of some degrees of success is investigated, various significant constraints are apparent. Notwithstanding its potential, fundamental knowledge in the multiphase flow simulations is still lacking because of its complexities, particularly in agitated vessels that have movable pieces. For example, CFD is still undeveloped to assess the nonhomogeneity impact and phase property changes in stirred polymerization reactors⁶. Besides, precision of some cases is maybe limited by low grid resolution^{11,12}. Even though Bakker's method¹³ tolerates bubble coalescence, a constant bubble dimensions is presumed. Another common limitation is that the impeller's condition where it is not directly simulated; using experimentally to determine impeller boundary condition. Similarly, no sufficient information available on such methods about the flow in the impeller area.

Thus in this study, the modelling techniques for gasliquid flow in agitated vessel is developed. This paper describes the development of the simulation technique for gas-liquid flow in the agitated vessels. The model is able to foresee the flow behaviour; mass transfer rate, interfacial area, gas holdup and reaction rates. This model has many applications in optimization and design of a widespread of gas-liquid industry.

2. Experimental

2.1 Modelling of Pitched-Blade Impeller

The flow is determined by separating the vessel into two domains in the Multiple Frames of Reference method⁸. In the impeller region, the flow is calculated in a revolv-

ing frame where the blade impeller is motionless; the velocities' alteration at the interface between two areas is made. Therefore, a steady-state calculation can be used. This single-phase flow's method can save a simulation time in 10 times with accuracy's level alike to the Sliding Mesh method⁷. Hence, for more effective computation simulation, this method is implemented in this study and extended to the two-phase flow.

In case of the construction model of the agitated vessel, the design of vertical cylindrical vessel with a flat site was chosen to run the simulation gas-liquid mixing. However, the simulation software to be used in this study is restricted to limitation use of Ansys[®] constraint. To obtain the gas-liquid mixing in the state optimum, the mechanical design and parameters need to be manipulated. The parameters will also be limited to an impeller blade's gradient, the number of impeller and the impeller rotation rate.

In this study, the pitched-blade impeller is used. Figure 1 shows three dimensions (3D) and side view of the pitched-blade impeller and its dimension as well. The pitched-blade impeller with 45° is designed by using DesignModeler[®] software. The details dimensions of the impeller is as follow; the total length of impeller, D = 0.5 m, the width of blade, W = 0.02 m, the diameter of center impeller; d = 0.03 and the distance between center impeller to the end blade; b = 0.025 m is shown as in Figure 1 below.

2.2 Modelling of Cylindrical Vessel

For the construction and modelling of the overall surface of agitated vessel model, DesignModeler[©] software is used. The details dimension of the vessel is shows as in Figure 2. In this experiment, the ratio of height over diameter vessel; H/T is equals to 2 will be used. Therefore, the height of the vessel, T is 2 m, the diameter of vessel, D is 1 m and the thickness of barrier, B is 0.01 m. This is because frequently the thickness of the barrier is chosen



Figure 1. Modelling of pitched-blade impeller in a 3D view and side view.



Figure 2. Design of overall surface agitated vessel model and blade impeller.



Figure 3. Mesh generation and defining finite volume grid in cylindrical coordinates and conditions restriction.

based on the 8-10% of vessel's diameter¹⁴. The position of the blade, *C* is set up about 1/5 ratio to the height of the vessel. The red arrow in Figure 2 shows the flow of nitrogen gas injected from a gas inlet at the underneath of the impeller and the bottom vessel.

2.3 Experimental Set-Up and Conditions

The choice of mixing media also plays an important role in these experiments. In this study, the mixing media has been restricted to the use of water as the liquid medium and nitrogen gas as the gas medium, and others related properties are set in the model. The vessel is baffled with a diameter of 1.0 m and a standard Rushton impeller 0.333 m diameter positioned at an allowance of 0.25 m. The gas flow rate is 0.00164 m³ s⁻¹ and the speed of impeller is fixed between 0 to 120 rpm. In order to determine and simulate a gas-sparged vessel for the distribution of bubble dimensions and local gas volume fraction, CFD model is set up.

There are three areas requiring breakdown namely region in the vessel (water), input (nitrogen gas) and impeller. For vessel's region, the fluid is water that has been set in a static state. For the pressure vessel, 1 atm is used with the assumption the vessel have the same pressure as pressure at the surrounding environment. The gravitational force is defined as at -9.81 ms⁻² on the *y*-axis and no temperature drop in the mixing process as well as no energy flow in and out of the system.

2.4 Mesh and Domain Generation

As shown in Figure 3, the vessel is designed by using a finite volume grid in cylindrical coordinates. All walls are assigned as no-slip boundaries to determine the distribution of velocity at nearby the wall, excluding a zero stress boundary is assigned for the liquid surface. The nitrogen gas is supplied at the sparger and released at the liquid surface.

2.5 Simulation Process

As all the boundary conditions are defined, the CFD simulation is run and the process is repeated with the step time of the data acquisition need to be scaled down due to the constraints of computer hardware. In order to determine the optimum condition for well mixing process, the CFD simulation is carried out by changing the parameter such as the impeller blade's gradient, the number of impeller and the impeller rotation rate. In this study, the range of impeller blade's gradient is between 0° to 90°, three number of impeller; impeller (a), (b) and (c) and the impeller rotation is between 90 to 120 rpm is used.

3. Results and Discussions

3.1 Image Reconstruction of Static Condition

The ability to predict the characteristic flow patterns for a Rushton impeller in an agitated vessel by using the CFD model is observed as shown in Figure 4. Along a cross-section through the central of vessel, the flow field demonstrations a characteristic pattern with radial discharge from the impeller. The gas nitrogen stream separates into upper and lower circulation regions, with liquid recurring axially to the uppermost and lowermost of impeller. A truncated velocity region perseveres away from the shaft and this region decreases with increasing the Reynolds number.

The difference in the color contour simulation results showed the difference of gas nitrogen density in water



Figure 4. Average image of the density of nitrogen gas mixing in the water.

after gas nitrogen was injected through the sparger that located at the bottom of center vessel. The distribution color range from blue which the highest density to the red color which is the lowest density of gas nitrogen distribution. The lowest density can be seen on the top of the vessel where circulation gas more focuses on the wall vessel.

Meanwhile, the highest density of the gas nitrogen was indicated at the bottom vessel as the gas inlet stream is located from the below the impeller where the impeller play an important role to push and distribute the inlet of the gas nitrogen to the whole vessel area. From the simulation result, the data simulation was interpolated into graph type as shown in Figure 5 where the highest value of the gas nitrogen density was $2.31 \times 10^{-1} \text{ mgl}^{-1}$ and the lowest value was $1.15 \times 10^{-2} \text{ mgl}^{-1}$.

3.2 Determination of Optimal Conditions for Well Mixing of Gas-Liquid

3.2.1 Gradient of Blades Impeller

In order to determine the best condition of the well mixing gas nitrogen in the agitated vessel, at first the gradient of blades impeller is changed at 0°, 30°, 60° and 90°. By exchanging the slope gradient of the blade impeller, the density of nitrogen gas in the distilled water is observed. The density of gas nitrogen in the dissolved water can be expressed in the tomogram image. In this study, 15 repetitions simulation were done where the gas nitrogen is injected simultaneously in the agitated vessel by changing the gradient of blades impeller between 0° and 90° in the static condition. Figure 6 shows the simulation result of gas nitrogen density in the dissolved water at the gradient of blades impeller between 0° to 90°. The density of gas nitrogen in the dissolved distilled water became



Figure 5. Density of gas nitrogen in 15 repetitions simulation at the gradient of blades impeller of 0° to 90°.



Figure 6. Image distribution of gas nitrogen's density in the dissolved water at the gradient of blades impeller between 0° to 90°.



Figure 7. Image distribution of gas nitrogen's density in the dissolved water with one impeller (a), two impellers (b) and three impellers (c).



Figure 8. Image distribution of gas nitrogen's density in the dissolved water at the rotation of blade impeller of 90, 100, 110 and 120 rpm.

stable after a while that shows the well mixing is slightly occurred in the vessel.

3.2.2 Number of Blade Impeller

Once the gradient of blades impeller at 60° was chose as the best gradient for the optimum condition, the simulation was continued by changing the number of impeller to select the advance well mixing condition for gas nitrogen in the dissolved water. Based on the height and the diameter of the agitated vessel, the maximum number of blade impeller can be used in this study is three. Figure 7 shows the result of image distribution of gas nitrogen's density with one impeller (a), two impellers (b) and three impellers (c). From the simulation, it shows the three numbers of impellers (c) gives the most appropriate condition for spreading of the gas nitrogen in the agitated vessel as three impellers give the optimum power to distribute and spread the nitrogen gas around the agitated vessel. The optimum power from the three impellers is able to withstand the movement of the nitrogen gas and pressure from water as well as be capable to distribute the gas around the agitated vessel.

3.2.3 Rotation of Blade Impeller

Based on the gradient of blades impeller at 60° and three number of pitched-blade impellers (c), the simulation was continued by changing the rotation of blade impeller to select the advance well mixing condition for gas nitrogen in dissolved water. Figure 8 shows the result of image distribution of gas nitrogen's density with the rotation of blade impeller is at 90, 100, 110 and 120 rpm. From the simulation, it shows the 90 rpm of rotation of pitchedblade impeller gives the most optimum condition for distributed and spread the nitrogen gas around the agitated vessel that shows in the red color. It is because the 90 rpm rotation of pitched-blade impeller can hold longer the nitrogen gas in the water comparing to others blade impeller's rotation. At the higher rotation; 110 rpm and 120 rpm, the blade impeller refused the stable and well mixing distribution of the nitrogen gas in the vessel as the greater rotation rate gives the powerful force and the interaction between the gas and water become unstable and turbulent flow. Besides, with the 90 rpm rotation of the blade impeller, it can save the energy without apply the higher blade impeller's rotation rate.

4. Conclusion

This study has focused on the use of CFD software to simulate the mixing of gas nitrogen gas in the dissolved water in the agitated vessel. The objective of this study is to investigate the optimum mixing conditions of a nitrogen gas dissolved in the distilled water by changing of the impeller blade's gradient, the number of impeller and the impeller rotation rate. In this study, the range of impeller blade's gradient was between 0° to 90°, three number of impeller; impeller (a), (b) and (c) and the impeller rotation is between 90 to 120 rpm is used. The reconstruction images of nitrogen-distilled water mixing in the agitated vessel are obtained from the Ansys® simulation. Based on the simulation result, the gradient of blades impeller at 60°, three number of impellers (c) and 90 rpm rotation of blade impeller, are chosen as the optimum condition for well mixing condition for gas nitrogen in the agitated vessel. These three parameters indicated the most appropriate condition for spreading of the gas nitrogen in the agitated vessel as he gradient of blades impeller at 60°, three numbers of impellers (c) and 90 rpm rotation of blade impeller give the optimum power to distribute and spread the nitrogen gas around the agitated vessel. The optimum power from three impellers is able to withstand the movement of the nitrogen gas and pressure from water as well as be capable to distribute the gas around the agitated vessel.

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