



Hydraulic Simulation of Bubble Flow in Bubble Column Reactor

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Abstract: Bubble column reactor are commonly used in a wide variety of applications, such as gas-liquid and gas-liquid-solid in plenty of chemical, petrochemical and biochemical industries. They supply many advantages while operating and maintenance such as high heat and mass transfer rates, compactness and low operating and maintenance cost. It is a critical to understand the complexity of the fluid dynamics in bubble column reactors due to its wide application in process engineering. This research shows the bubble column flows and provides mean velocity profile for columns operated over a wide range of superficial velocity, operating pressure, physical properties, and column diameter. The possible ways to conduct such research is by performing the experimental method and software simulation method. The experimental setup is usually expensive to run, while the software simulation by using computational fluid dynamics (CFD) is an alternative approach to evaluate the characteristics of bubble column reactor and it cost less than the experimental measurements.

Keywords: Bubble column, CFD, fluid mixing

1. Introduction

A bubble column reactor (BCR's) is a cylindrical vessel that has a gas distributor at the bottom of the vessel. The gas is sparged in the form of bubbles into either a liquid phase or a liquid-solid suspension. BCR's is one of the division of multiphase reactor which include the trickle bed reactor, fluidized bed reactor and bubble column reactor. Multiphase flow takes place when more than one phase appears in a flow field and the phases appear in different physical states of matter or appear in the same physical state of matter but with distinct chemical properties. The phases occurred in multiphase flow are often determined as belonging to the primary or secondary phases. The primary phase is described as the phase that is continuous about, or enveloping of, the secondary phase. The secondary phase is thought to be the material that is distributed throughout the primary phase. Each phase present in multiphase flow may be either laminar or turbulent, which introduce to a classified of potential flow regimes for multiple phases in the same channel.

BSR's has been exploited in chemical, petrochemical, biochemical and metallurgical industries. They are employed in chemical reaction processes for instance the aeration of fermentation broths as in the production of penicillin, polymerization, carbonation of lime slurry, alkylation, chlorination of paper stock, production of citric acid from sugar by action of microorganisms, hydrogenation of vegetable oils and oxidation, and in biotechnology processes such as antibiotic fermentation, single protein production and

animal cell culture and in the manufacturing of synthetic fuel by gas conversion process. Other usage includes biological waste water treatment [1].

Table 1 – Industrial related in bubble column reactor [2]

	Temperature, °C	Pressure, atm (MPa)
Partial oxidation of ethylene to acetaldehyde	130	3 (0.3)
Wet-air oxidation of sewage sludge	200 – 300	40 – 120 (4 – 12)
Oxidation of cumene to phenol	80 – 125	5 – 8 (0.5 – 0.8)
Hydroxylamine formation by hydrogenation	50 – 60	25 – 30 (2.5 – 3)
Conversion of natural gas to liquid fuels via syngas	900	15 – 30 (1.5 – 3.0)
Methanol synthesis	(1) 350 – 400 (2) 220 – 250	(1) 250 – 350 (25 – 35) (2) 50 – 100 (5 – 10)
(1) BASF (2) Eastman Chemicals, Air-Product, DOE		
Fischer-Tropsch synthesis	220 – 260	136 – 204 (13.6 – 20.4)
Hydroformylation (Oxo) processes	160 – 200	50 – 100 (5 – 10)

Bubble column reactor offers distinctive advantages in both design and operation compared to other reactors. For instance, the simplicity of their construction and the lack of any mechanical moving parts are applicable for high pressure operating conditions. In addition, BCR's provides a good heat and mass transfer characteristics which suites in operating the reactor at close to isothermal conditions, and powerful mixing between the gas and liquid phases with low energy consumption. At the same time these types of reactors are cheaper and require less floor space, and can easily accommodate slow reactions due to high liquid residence time [3].

However, it is highly important to understand the concept of the hydrodynamic of bubble column due to its operation that determined by several criterions such as superficial gas velocity, gas sparger design, gas holdup distribution, gas-liquid mass and heat transfer coefficients, bubble rise velocities and bubble size distributions, additionally, bubble size distribution and bubble velocity distribution are key parameters to assess the drag forces on bubbles and in using the bubble population balance in Computational Fluid Dynamics (CFD) [4]. Despite the fact of the mechanical designing of bubble columns without internals is not difficult, their hydrodynamics is still complicated and the understanding required of their various parameters that affect the bubble column performance.

The critical need to understand the complexity of the fluid dynamics in bubble column reactors due to its wide application in process engineering. CFD simulation is useful for a variety of gas-liquid dispersion problems including bubble column which offer a cheaper but with a faster solution compared with measuring using experimental. Hence, the main objective of this project is to investigate the gas holdup, and velocity profile on hydrodynamic behavior of bubble column reactor with different grid resolution by numerical approach. The simulation that will be use is based on two-fluid model and the approach used in this simulation work is the eulerian-eulerian approach. The $k-\epsilon$ mixture turbulence model was utilized to assure the effect of turbulence. Finally, the analysis that will carry out includes gas hold-up and gas velocity on hydrodynamic behavior.

2. Fluid Hydrodynamics and Regime Analysis

One of the method to characterize the hydrodynamics in bubble column reactor is by flow regimes, due to superficial gas velocity, flow regimes can be divided into three categories which are the homogenous regime, transition regimes and heterogeneous regimes [5]. The homogeneous regime exists at low superficial gas velocities and changes to the heterogeneous regime with an increase in the superficial gas velocity. The effect of different range of flow regime can clearly be seen on the hydrodynamics, heat and mass transfer, and mixing behavior. It is therefore extremely important to understand the different hydrodynamics and flow regime transitions for the purpose of reactor design, operation, control, and scale-up.

When flow structures change, the performance of bubble column changes. The heterogeneous regime is required in most industrial reactors, whereas the homogeneous flow regime is desired in some bioreactors [6]. There is research that conducted an experiment on that which is used gas holdup and pressure fluctuation analysis to identify flow regimes in a slurry bubble column [7,8]. The results noticed that when the gas velocity under 0.05m/s a free bubbling regime pattern appeared, but while the gas velocity is above 0.125m/s a gross recirculation pattern is observed. Another research [9] used a slurry bubble column and employed statistical and chaotic parameters to analyze computed tomography data. The average absolute deviation is a tool of time domain analysis, and use of the Kolmogorov entropy connotes state space analysis. Results showed that nonlinear chaos analysis can be successfully applied to compute tomography data for the identification of various flow regime boundaries.

2.1 Gas Holdup

Gas hold-up plays a significant role in the hydrodynamic parameters that influence in the design, development scale-up and troubleshooting of bubble column reactor system. Gas hold-up is the volume fraction of gas phase employed by the gas bubbles. It is a dimensionless parameter of bubble column reactor design that describe the transport development of bubble column system [10]. The relationship between the volume fractions of gas and the gas holdup in bubble column reactor which can expressed as $\Delta P = (\rho_{eg} + \rho_{el} + \rho_{es})g\Delta H$ where ΔP is the static pressure drop, ρ_{eg} , ρ_{el} , ρ_{es} are the volume of gas (gas hold-up), liquid and solid phases, g is the gravitational acceleration and ΔH the density and height difference between the transducers terminals. [11].

There are many factors that affected gas hold-up such as solid phase properties, column dimensions, gas distributor design, operating temperature and pressure, superficial gas velocity, and liquid properties [12]. Therefore, several assumptions had been made in the simulation for the purpose to understand the behavior of the bubble in the column reactor for the first simulation work.

2.2 Gas Velocity

In designing and operating of bubble column reactor, there are many parameters that effect the efficiency of the associated process. One of these parameters is gas velocity. Gas velocity is the gas volumetric flow rate divided by the column cross sectional area. There are many conducted experiments concerning to the various hydrodynamic aspect of the different flow regime, one in these experimental investigation is by Tang and Fan [13,14] concluded that with the increasing of liquid velocity will effect volumetric mass transfer coefficient by increasing it, while the affection on the gas hold-up is only slightly increased.

Yeng and Chaumat [15,16] resulted the increase in gas hold-up influenced by the increase in liquid velocity. They also found that the turbulence induced by liquid flow will enhance mass transfer at higher liquid velocity, while Hyndman [17] identified the flow regime transition, where he plotted the gas hold-up α_g with the respect to gas velocity U_g . The results show that in the homogenous regime, the gas hold-up is almost linear and it will increase with the increment of gas velocity, but when the flow enters the heterogeneous regime, the increment of gas velocity and gas hold-up becomes less pronounce. Moreover, the identification of flow regime can be indicated by using the slope of α_g-U_g plot.

3. Euler-Euler (two-fluid) Approach

Euler-Euler approach consider the two interpenetrating continua methods which are the continuous and dispersed phases. To characterize the motion of phases, the two-fluid model was implemented. From the mathematical point of view, the macroscopic description of both phases is derived by ensemble averaging the fundamental microscopic conservation equations for each phase, the flow description consists of differential equations describing the conservation of mass, momentum and energy for each phase separately. The mass balance is given by (in absence of interphase exchange),

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \nabla(\alpha_k \rho_k u_k) = 0 \quad (1)$$

$$\sum_{k=1}^n \alpha_k = 1 \quad (2)$$

where α is the volume fraction, ρ is density and u is the velocity of each phase. k is the phase indicator, $k=1$ for the liquid phase and $k=2$ for gas phase. The corresponding momentum equations for the two phases can be written as,

$$\frac{\partial(\alpha_k \rho_k u_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k u_k) = -\alpha_k \nabla p + \nabla \cdot (\alpha_k \tau_k) + \alpha_k \rho_k g + (-1)^k F_{exchange} \quad (3)$$

where $k=1$ for continuous phase and $k=2$ for dispersed phase. τ is the effective stress tensor which contains not only the contributions from viscous effects but also the contributions from the cross-correlations between velocity fluctuations arising from the averaging, $F_{exchange}$ is the interfacial force, which explicitly contains the mean interaction between the phases and accounts for the effects of two-way coupling, and ρg is the gravity force.

In most industrial applications, high gas superficial velocity is used which results in heterogeneous flow regime, i.e., the so-called churn turbulent flows. Under such conditions Euler-Euler method is usually preferred. As stated above, in the Euler-Euler approach the information regarding the microscopic scale has been lost leading to the closure problem which is the key issue of the Eulerian two-fluid model.

4. Results and Discussion

A simulation of bubble column reactor with height of 0.96 m and diameter of 0.19 m. The achieved results will be revealed graphically in this chapter by using Computational Fluid Dynamic Ansys FLUENT 15. The simulation of gas phase transport in a primary liquid phase was performed through the influence of fluid transport models that have on the motion of gas and liquid mixtures of k-epsilon turbulence models. While simulating the bubble column reactor profile, the motion of the gas phase through the liquid-phase is highly unstable, it would be appropriate to use time dependent formulations of the transport equations as the turbulent nature of the flow is important to the inclusion of models. From the unsteady nature of the flow it is necessary to consider the discussion of time averaged variables such as the vertical velocity.

4.1 Volume Fraction

Contours of volume fraction profiles for air velocity of course mesh are displayed in Fig. 1. During the simulation process the volume fraction profiles alters with the increasing of time step. However, after some period there is no critical alteration in the volume fraction profiles. This illustrate that the bubble column has reached the quasi steady state. It has been observed that the increasing of volume fraction profiles is directly proportional to the increasing of gas velocity. The volume fractions of gas are not characterizing uniformly and it is highly time-dependent.

Fig. 2 shows the contours of volume fraction profiles for air velocity of fine mesh. The resulted contours of the volume fraction with meshing size of course mesh is thicker than the resulted contours volume fraction with fine mesh. While the radial volume fraction of fine mesh is much clearer than the volume fraction of course meshes, that could be explained the higher grid resolution. On other hand, the gas volume fractions are much lower near the wall than in the column bulk. However, it seems that both grid resolutions has same volume fraction.

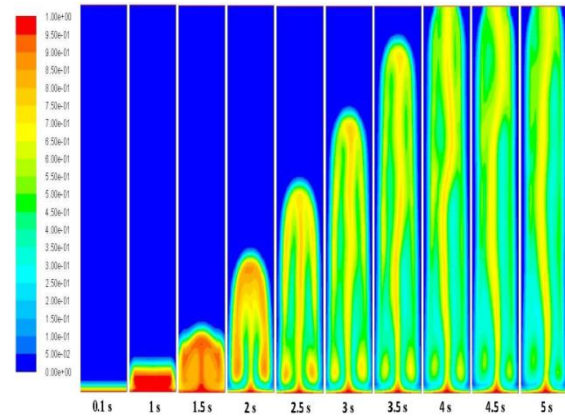


Fig. 1 - Contour of the instantaneous volume fraction of course mesh

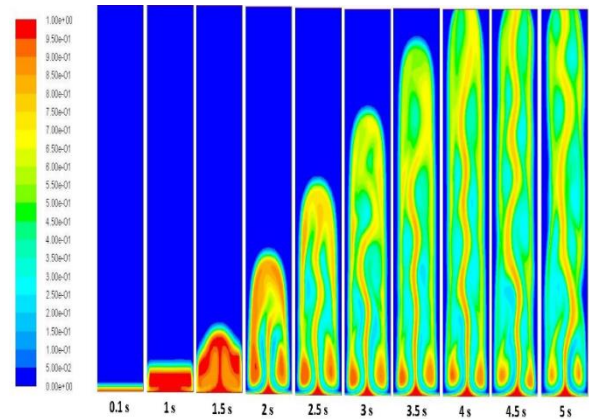


Fig. 2 - Contour of the instantaneous volume fraction of fine mesh

4.2 Gas Holdup

Gas holdup is considered as crucial criterion that controls the liquid recirculation in bubble column reactor operation and can be described as fraction of gas-liquid volume occupied by gas. Gas holdup is also able to be obtained by a point in the column or either by the average value over the entire reactor. It has been earlier well recognized that the gas superficial velocity, is the essential variable that influence gas holdup profiles and that increased leads to higher gas holdup.

Fig. 3 illustrated the relationship between radial gas holdup profile with superficial gas velocity. For the course mesh, it is clearly that there is a slow raising of gas holdup from point (0.22, 0.05) to the point (0.32, 0.35), but from point (0.32, 0.35) to the point (0.67, 0.55) where it moves rapidly raising the gas holdup and the air velocity. However, at point (0.67, 0.55) to the point (0.95, 1.1) the slope of gas hold up is gradually increasing with air velocity. Finally, it can be seen that these two distributions match well, except there is a little higher probability at gas holdup intervals between gas hold up for the course mesh and gas hold up for the fine mesh. This is because the grid resolution affects the results of two volume fraction obtained.

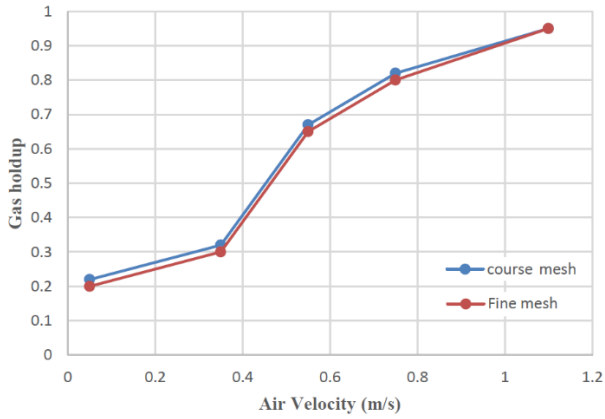


Fig. 3 - Gas holdup vs. air velocity

4.3 Gas Velocities

The gas velocity is one of the key operating variables that affects the hydrodynamics in bubble columns. In CFD simulations of gas velocity in bubble column reactor, an inflow boundary condition is to be subjected from the bottom gas distributor. Which is specified as having a uniform gas velocity corresponding to the described gas velocity, implicitly assuming that the pressure drop through the gas distributor is high. The velocity varies with time and location in bubble column reactor. Contours of radial velocity profile of air with course mesh are visible in Fig. 4. From the figure, it was found that radial velocity profiles are developed with increasing of time intervals during the simulation of bubble column reactor. The alteration of radial velocity profiles is from 1 second to 5 seconds. According to the results obtained, the variation of the radial velocities has a maximum of 1.4 m/s and minimum of -1.36 m/s.

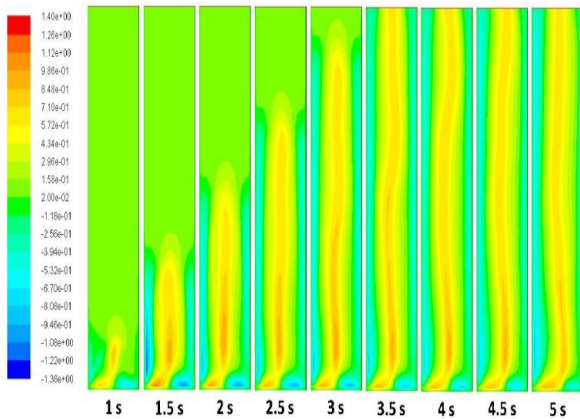


Fig. 4 - The contours of radial velocity of course mesh

Fig. 5 shows the contours of radial velocity profile of air for fine mesh. In accordance with the results obtained, the variation of the radial velocities has a maximum of 1.40 m/s and minimum of -1.36 m/s. The similarity between these two mesh sizes is the result of the fact that radial velocity profiles and time intervals are strongly correlated. While the dissimilarity between the two meshes that in fine mesh, a slight of turbulence effect is observed. Speaking generally, an increase in time intervals leads to an increase in radial velocity profiles.

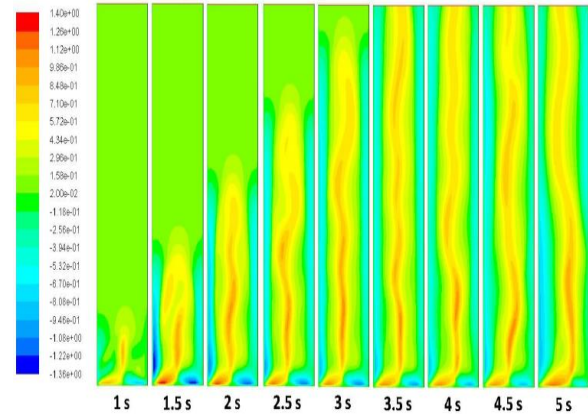


Fig. 5 - The contours of radial velocity of fine mesh

The vector of velocity magnitude is helpful to regulate the flow pattern. Fig. 6a shows the vector of velocity magnitude of air and its direction for the course mesh while Fig. 6b illustrate the vector of velocity magnitude of and its direction for the fine mesh. The variation of velocity in between 0.12 m/s to 0.122 m/s at the outlet. It is found the gas velocity to be higher at the top part than in bottom part. The velocity seems to have an equal speed over the cross section due to the assumption of the uniform inlet velocity. However, it can be seen that course mesh have less vector velocity along the column than fine mesh due to the difference of grid resolution.

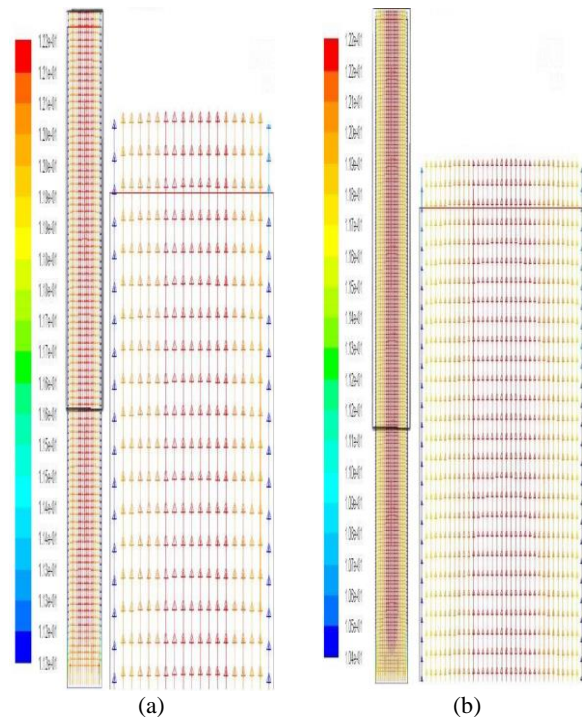


Figure 6. (a) Velocity vectors by the vector magnitude for course mesh. (b) Velocity vectors by the vector magnitude for fine mesh.

4.4 Pressure

Pressure is considered one of the key parameters used to analyses the flow hydrodynamics in gas-liquid multiphase reactor. The contours of static pressure at 5 seconds of time for course mesh is displayed in Fig. 7a. Meanwhile, the contours 5 seconds of time of static pressure for fine mesh is presented in Fig. 7b. It can be seen from that the maximum

pressure is 6210 Pa and the minimum pressure is -79.6 Pa. In general, we can conclude that the pressure at the inlet is high, while it is decreasing gradually when moving toward the outlet. Besides that, the determination of pressure at inlet and outlet is significant in finding the pressure drop across the column.

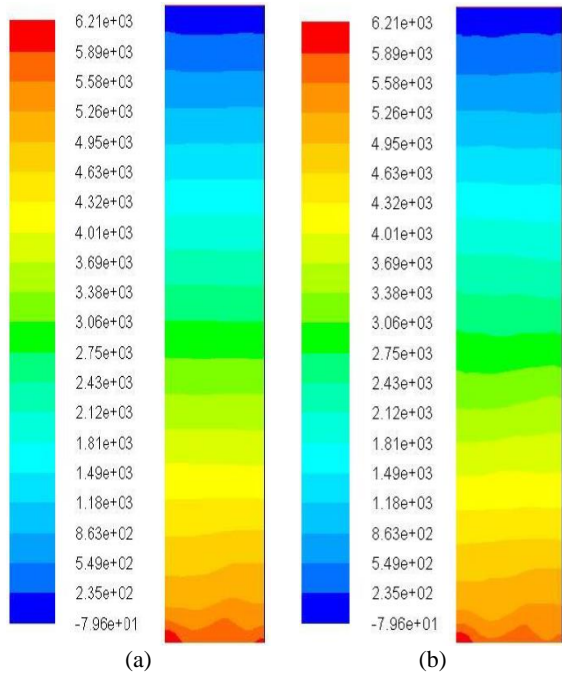


Fig. 7 (a) Contours of static pressure for the course mesh. (b) Contours of static pressure for the course mesh.

The plot shown in Fig. 8 illustrate the static pressure at 0.5 m height of column for the time of 5 seconds, the plot shows the fine mesh line and course mesh line, it can be seen that the two lines are intersecting and have almost the same value of range. On this plot, the maximum value is 2665.43 Pa of static pressure for the course mesh and the minimum of -31.8893 Pa of static pressure. While the static pressure of fine mesh has a maximum of 2602.06 Pa, and minimum of -54.4341 Pa. these deviation of values between fine mesh and course mesh can be explained by the difference of grid resolution.

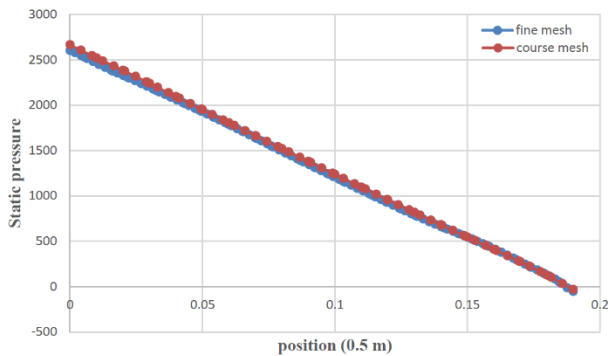


Figure 8 - Static pressure vs. column height of 0.5 m.

The relationship between the magnitudes of the pressure drop along with the heights bubble column reactor where the pressure drop is higher at the inlet is illustrated in the plot from Fig. 9. These figure were plotted to define the pressure at different heights of both course mesh and fine mesh of the column. For this plotted graph, the course mesh has maximum

static pressure of 1476.93 Pa and a minimum of -31.8893 Pa. On other hand, static pressure for the fine mesh has a maximum of 1468.43 Pa, and with minimum of -54.4341 Pa. these results can be described that the pressure is descending progressively along the column.

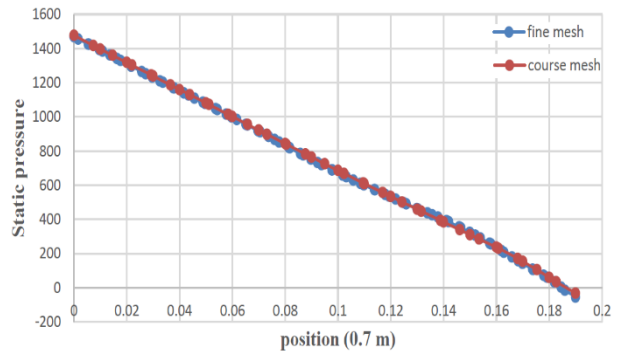


Fig. 9 - Static pressure vs. column height of 0.7 m.

5. Conclusion

In this study, the gas-liquid hydrodynamics flow for the bubble column reactor with width of 0.19 m and height of 0.96 m. by using different grid resolution to investigate its affection to hydrodynamic behavior. Different criterion has been studied consist of volume fraction, gas hold up, gas velocities and pressure. The Eulerian-Eulerian methods is used with mixture multiphase model. A standard k-epsilon mixture multiphase model is used to model turbulence with standard wall function. According to the results, it has been observed that the increasing of volume fraction profiles is correlated with the increasing of time step. The effect of different grid resolution on volume fraction is found that the smaller of grid resolution the clearer and less thickness are observed. The variation of the gas holdup is from 0.22 to 0.95 for the grid resolution of 0.01 m, and for the grid resolution of 0.005 varies from 0.2 to 0.95, the deviation of 0.02 can be explained of the cause of different mesh sizes. The magnitude of vector velocity varies in between 0.12 m/s to 0.122 m/s at the outlet for the two mesh sizes. It is found that contours of radial velocity profiles are developed along with increasing of time intervals. At lower mesh size, the radial velocity profile becomes narrow due to an increase grid resolution. The relation of pressure drop along with height of bubble column is that the pressure is high at the inlet then it gradually descending in the direction of the outlet.

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