Computational flow analysis of bubble formation dynamics in a liquid column subjected to high centrifugal force

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Abstract. Bubbling of gaseous medium in a liquid column is integral to many multiphase process reactors involving liquid phase and gas phase reactants. In one such reactor called centri-bubble singlet oxygen generator (CBSOG), chlorine gas is injected against a substantively high centrifugal force into a layer of basic hydrogen peroxide (BHP) solution. This process generates small bubbles that facilitate the reaction between chlorine gas and BHP solution at the gas liquid interface, resulting in the production of singlet oxygen. Performance of this device depends primarily on bubble formation time, its shape and size, and its interaction with other bubbles. This paper presents the numerical analysis of bubble formation at high centrifugal force (3800 m/s²) for various gas flow rates at orifice sizes of 0.3mm and 0.5mm. The volume of fluid (VOF) model of the computational flow dynamics (CFD) solver Fluent has been used for the computations to carry out a transient 3-dimensional simulation for generation of bubbles in a laminar incompressible flow.

Key Words: Bubbling; VOF; CFD; CBSOG.

1. Introduction
When a gas stream is injected through an orifice into a liquid column, either bubbling or jetting flow regimes may occur. In the bubbling regime, the dispersed gas moves inside liquid as discrete bubbles, while in jetting regime the gas penetrates through the liquid column and moves as a continuous jet. It is expected that the working of CBSOG device will be better and BHP aerosols generation will be lesser in the case of bubbling regime. Payne and Prince [1] studied bubble to jet transition in a single submerged orifice, and proposed a correlation for the ratio of liquid height ($H$) and orifice diameter ($d_n$) in terms of a modified Froude number,

$$\frac{H}{d_n} > 1.5 \left( \frac{u_l^2 \rho_g}{d_n \rho_l} \right)^{0.5}$$  

(1)

In the bubbling regime the breakdown of the balance of forces acting on the bubble induces the detachment of the bubble from the nozzle. For zero liquid cross velocity $u_l=0$ and subsonic flow of gas the detachment radius of the single bubble is given by the following correlation [2],
Here, $U_g$ is the gas inlet velocity, $G$ is centrifugal acceleration, $\rho$ is the density and $\mu$ is viscosity with subscripts ‘g’ for gas and ‘l’ for liquid.

It can be observed from the above equation 2 that increase of the orifice diameter results in increase of the generated bubble size at the same gas velocity and other parameters.

2. Volume of Fluid model

It is a challenging task to numerically compute two phase flow with moving interface. The shape and movement of the interface and the geometric configuration of each phase needs to be computed as part of the solution. The large property changes also add to the complexity of the problem. In a recent numerical study by K. Andrzej et al [3] commercial CFD solver Fluent has been used for simulating bubble formation process in a low viscosity system (air-water). The simulations were done using volume of fluid (VOF) method and the results compared satisfactorily with the experimental data.

The volume of fluid (VOF) model directly determines the motion of all phases thereafter the motion of the interface is indirectly deduced. The motion of the different phases is tracked by solving a continuity equation for the volume fraction of each phase. The volume fraction for a particular fluid inside a cell is defined as its material volume divided by the total cell volume.

The VOF algorithm consists of three major steps, the interface reconstruction, which determines the interface in each cell based on volume fractions, the advection algorithm, which calculates the distribution of volume fraction at the next time step by solving an advection equation, and the surface tension model, which takes account of surface tension effects at the interface. The advection equation for void fraction $\alpha$ is as under:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{V}) = 0$$

3. Numerical Model

The 3-D computational domain used in the simulation is shown in Figures 1 and 2. It has a cubical shape with dimensions being 8mm ($x$) x 9mm ($y$) x 6mm ($z$) for 0.3mm orifice case and 8mm ($x$) x 13mm ($y$) x 8mm ($z$) for 0.5 mm orifice case respectively. There are two orifices on one of the face and gas will flow through these orifices inside the domain along the x-direction.

The different physical properties of gas and BHP used in the simulations are tabulated below.

| Properties             | Gas     | BHP    |
|------------------------|---------|--------|
| (In SI unit)           |         |        |
| Density (Kg/m$^3$)     | 1.225   | 1250   |
| Viscosity (Kg/m-s)     | 1.7894e-05 | 0.02   |
| Surface Tension (N/m)  | 0.050   |        |
These solution parameters were selected for accuracy and better convergence.

Momentum Equation: First order upwind
Pressure: PRESTO
Pressure Velocity Coupling: PISO
Volume fraction: Geometric-Reconstruct
Residual: $1 \times 10^{-6}$ (For all equation)

The restrictions imposed due to the Courant Fredrich and Levy (CFL) condition, gravity and surface tension gives the estimate of the maximum time step for proper numerical stability.

$$\Delta t \leq \left( \frac{\Delta x}{U}, \frac{\Delta x}{\sqrt{2g\Delta x}}, \sqrt{\frac{\rho}{4\pi\sigma \times \Delta x^{1.5}}} \right)$$

Here $\rho$ is the average density of the two fluids and $\sigma$ is the surface tension. In the above three conditions the surface tension criteria is the most stringent criteria when the fluid velocity is low. Thus, for a 60 micron size cell and given gas-BHP pair the above conditions result in $\Delta t \leq 1.5 \times 10^{-5}$.

4. Results and Analysis
These simulations illustrated the process of bubble formation in a stagnant liquid from orifices of 0.3mm and 0.5 mm diameters at different mass flow rate of gas. The boundary condition at orifice has been set as mass flow inlet. The face opposite to the orifice has been set as pressure outlet. All other faces have been designated as wall. Also, a centrifugal acceleration of 3800 m/s$^2$ has been applied in the negative X-direction. The solution is assumed converged when the residual value falls below $10^{-6}$ for all the equations. Table 2 shows the Reynolds number of the flow at the orifice for different flow rates and orifice sizes.
Table 2. Reynolds number of flow at different flow rates.

| Mass Flow rate (x10^-6Kg/m²) | Gas Volume (CC/min) | Reynolds no | Mass Flow rate (x10^-6Kg/m²) | Gas Volume (CC/min) | Reynolds no |
|-------------------------------|---------------------|-------------|-------------------------------|---------------------|-------------|
| 2.75                          | 134.7               | 652.25      | 538.8                         | 11                  | 1565.4      |
| 5.5                           | 269.4               | 1304.5      | 808.2                         | 16.5                | 2348.1      |
| 8.25                          | 404.1               | 1956.75     | 942.9                         | 19.25               | 2739.45     |
| 11                            | 538.8               | 2605        | 1077.55                       | 22                  | 3130.8      |
| 14.5                          | 710.2               | 3439.14     | 1346.94                       | 27.5                | 3913.5      |
| 16.5                          | 808.2               | 3913.5      | 1616.33                       | 33                  | 4696.2      |
| 19.25                         | 942.9               | 4565.75     | 1885.71                       | 38.5                | 5478.9      |

4.1 Case-1: 0.3mm orifice size

The simulations have been carried out with a time step of 1µs (much less than the requirement from the CFL criteria) for six different mass flow rates of the gas through each orifice viz., 2.75µKg/s, 5.5µKg/s, 8.25µKg/s, 11 µKg/s, 16.5 µKg/s and 19.25 µKg/s. The gas velocity at the orifice inlet is around ~29 m/s for 2.75µKg/s and it increases to ~200 m/s for the flow rate of 19.25 µKg/s. Thus, in all the cases the flow velocity is much less than the sonic speed (~330m/s) and hence the assumption of incompressible flow is justified.

It is seen that at 2.75µKg/s (through single orifice) the gas flow is perfectly in bubbling regime. However, as the flow rate is increased to 19.25µKg/s per orifice it starts to show characteristics of jetting flow. The following table shows the bubble diameter (spherical equivalent) at different flow rates at the time of detachment and also as estimated from available correlations.

Table 3. Bubble diameters (0.3mm orifice size).

| Flow Rate per orifice (µKg/s) | Detached Bubble Diameter (mm) | Bubble Diameter From Correlation (mm) |
|------------------------------|-------------------------------|---------------------------------------|
| 2.75                         | 1.7                           | 1.84                                  |
| 5.5                          | 2.22                          | 2.3                                   |
| 8.25                         | 2.34                          | 2.6                                   |
| 11                           | 2.48                          | 2.86                                  |
| 16.5                         | -                             | 3.26                                  |
| 19.25                        | -                             | 3.4                                   |

The bubble detachment time decreases with the increased gas flow. Figure 3 shows the bubble position after detachment for different flow rates. Detachment time has decreased from 1.4ms to 0.9 ms as the flow rate increased six times. Bigger bubbles are expected to move faster inside the liquid after detachment due to higher buoyancy force. Thus at higher flow rate the overall gas residence time inside the liquid will be less.
Figure 3. Bubble detachment at different flow rates (0.3mm orifice).

Figure 4. Comparison of Bubble diameter as obtained from simulations and correlation.
It can be deduced from the figure 3, that gas flow is completely in bubbling regime till the mass flow rate of 11 μKg/s. At the flow rate of 16.5 μKg/s there is no clear cut separation of two bubbles and at 19.25 μKg/s there is clear sign of jetting. Thus for given flow conditions the fully bubbling regime can be expected for mass flow rate lower than 16.5 μKg/s. Also at lower flow rate the bubble shape is expected to be more smooth and regular. The plot in figure 4 compares the detached bubble diameters as obtained from simulation and theoretical estimation for different flow rates. The maximum deviation in diameter values (between theoretical estimate and simulation result) is of the order of 13%. Thus it can be said that both the simulation and correlation results are in fair agreement with each other.

4.2 Case II: 0.5mm orifice size

The simulations have been conducted again with a time step of 1 μs (much less than the requirement from the CFL criteria) for six different mass flow rates of the gas through each orifice viz; 11 μKg/s, 16.5 μKg/s, 22 μKg/s, 27.5 μKg/s, 33 μKg/s and 38.5 μKg/s. The gas velocity at the orifice inlet is around ~46 m/s for 11 μKg/s and it increases to ~160 m/s for the flow rate of 38.5 μKg/s. Thus, in all the cases the flow velocity is much less than the sonic speed (~330 m/s) and hence the assumption of incompressible flow is justified.

It is seen that at 11 μKg/s (through single orifice) the gas flow is perfectly in bubbling regime. However, as the flow rate is increased to 33 μKg/s per orifice it starts to show characteristics of jetting flow. Figure 5 shows the shape, size and position of the bubble after detachment for different flow rates. It is clear that bubbling regime exists till 27.5 μKg/s of flow rate and after that there is clear sign of jetting. Thus for a 0.5 mm orifice size the maximum flow rate that can be used within bubbling regime is of the order of 27.5 μKg/s.

The following table gives the bubble diameter (spherical equivalent) at different flow rates after the detachment and also as obtained from available correlations. It is evident that when the flow rate is increased by ~3.5 times there is an increase of ~1.5 times in the bubble diameter.

| Flow Rate per orifice (μKg/s) | Detached Bubble Diameter (mm) | Bubble Diameter from Correlation (mm) |
|-------------------------------|-------------------------------|--------------------------------------|
| 11                            | 2.6                           | 3.16                                 |
| 16.5                          | 3.24                          | 3.61                                 |
| 22                            | 3.57                          | 3.95                                 |
| 27.5                          | 3.74                          | 4.25                                 |
| 33                            | -                             | 4.5                                  |
| 38.5                          | -                             | 4.73                                 |

The plot in figure 6 compares the detached bubble diameters as obtained from simulation and theoretical estimation for different flow rates. The maximum deviation in diameter values (between theoretical estimate and simulation result) is of the order of 18%. Although the qualitative prediction are in agreement, however it seems that the correlation over predicts the bubble diameter. The same was also observed in the predictions made using correlation in the case of 0.3 mm orifice.
Figure 5. Bubble position and detachment at different flow rates for 0.5mm orifice.

Figure 6. Comparison of Bubble diameters as obtained from simulation and correlation.
5. Conclusions
Definite inferences may be drawn from detailed computational analysis with regards to the bubble generation mechanism and its traverse inside a stagnant BHP column anchored under a substantively high centrifugal force (3800 m/s²) condition. It is evident that high flow rates are associated with larger bubble diameter and diminished detachment time. The rate of increase of bubble diameter is steep at lower flow rates but decreases at higher flow rates. The bubble shapes are more regular and smooth at lower flow rates whereas higher flow rates bubbles tend to be elongated and non-regular.

Bubble size is a strong function of flow rates and a relatively weak function of orifice size. In the investigated cases where the inter orifice spacing is ~10d the bubbling regime there is no collapse or coalescence of adjacent bubbles. In the two cases examined, for 0.3mm orifice the maximum flow rate for bubbling regime is ~11μKg/s and for 0.5mm orifice it is ~27.5μKg/s. Further, it may also be inferred that available correlations developed at gravity or low centrifugal force conditions for bubble formation and detachment are in qualitative agreement with numerical results obtained at high centrifugal force conditions albeit with mild over prediction of bubble diameters.

6. References
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