Simulation of gas-liquid bubble column contactor using OpenFOAM

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Abstract

The objective of the present study is to numerically Simulate the gas-liquid bubble column contactor using the open source CFD package OpenFOAM. This report helps the reader to understand the step-by-step procedure involved in simulating bubble column contactor and explains the details regarding the boundary conditions, solver settings etc. Geometry and mesh have been generated using 'blockMesh' utility available in OpenFOAM and flow has been simulated using "twoPhaseEulerFoam" solver. Three different velocities have been considered in this case (0.2m/s, 0.4m/s and 0.6m/s).

1. Introduction

- Bubble Column is a type of chemical process equipment used to promote mass transfer between a gas and a liquid. These devices are generally designed to maximize the contact surface area and interaction time between the two phases, enabling efficient transfer of a component like absorption, mixing, or chemical reaction from one phase to the other.
- Gas-liquid reactors are commonly used in various industrial applications. Examples of industrial applications like
  - Hydrogenation
  - Chloration
  - gas absorption processes
- A bubble column usually takes the form of a cylindrical tank with aspect ratios between 2 and 10.
- The gas is injected at the bottom of the column through a sparger into the continuous liquid.

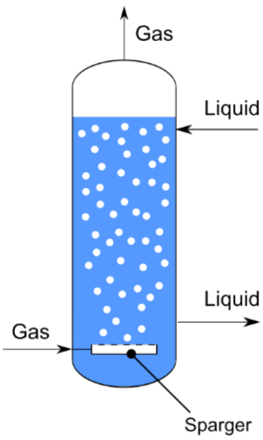

Figure 1: Bubble Column [20]

- Advantages of Bubble Column Contactor-
  - High Heat and mass Transfer Rates
  - Proper Mixing of the Substances
  - Low cost of Maintenance
  - It is Simple to Operate because of no moving parts
  - It is suitable for slow reactions
  - Highly Versatile

2. Problem Statement

Study and simulate the effect of velocity in the 2D rectangular gas liquid bubble column under laminar conditions.

3. Mathematical Approach: -

- Bubble column reactor is a multi-phase flow because 2 distinct physical phases (gas and liquid) are flowing simultaneously in the domain.
- Two types of mathematical approaches can be used:
    - Eulerian – Eulerian approach
    - Eulerian – Lagrangian approach
- In this case Eulerian – Eulerian approach is used because it treats both the continuous (liquid) and dispersed (gas) phases as **interpenetrating continua** rather than tracking individual particles.
- Eulerian multi-phase models can account for **dispersed – continuous** phase interactions and **continuous – continuous** phase interactions.

3.1. Eulerian – Eulerian-

- In this model, the two different phases in a multiphase flow are assumed to be mathematically interpenetrating continua and these phases have the same flow pressure. Interpenetrating continua defines the volume fraction volume occupied by the phases in the given domain.
- The following Governing equations are solved for each phase
    - Conservation of mass for a phase

$$\frac{\partial(\alpha_k \rho_k)}{\partial t} + \nabla.(\alpha_k \rho_k u_k) = \sum_{j=1}^{N} (\dot{m_{jk}} - \dot{m_{jk}}), \qquad (1)$$

(Sum of volume fraction is unity), $\sum_k \alpha_k = 1$

α = volume fraction, ρ = density, u = velocity, N = totoal no of phases
$\dot{m}$ = mass transfer rate

- Conservation of momentum for a phase

$$\frac{\partial(\alpha_k \rho_k u_k)}{\partial t} + \nabla.(\alpha_k \rho_k u_k u_k) = -\alpha_k \nabla P + \alpha_k \rho_k g + \nabla.\alpha_k(\tau_k + \tau_k') + M_k \qquad (2)$$

P = pressure, M = sum of interfacial forces (lift, drag, virtual mass) and momentum transfer associated with mass transfer

$$M = F_D + F_{TD} + F_L + F_{VM} + \sum_{j=1}^{N} (\dot{m_{jk}} u\_j - \dot{m_{jk}} u\_k) \qquad (3)$$

- Conservation of energy for a phase

$$\frac{\partial(\alpha_k \rho_k h_k)}{\partial t} + \nabla.(\alpha_k \rho_k u_k h_k) - \nabla.\left[\alpha_k \left(\lambda_k \nabla T_k + \frac{\mu}{\sigma_h} \nabla h_k\right)\right] = Q_k \qquad (4)$$

$$h = \text{enthalpy}, \lambda = \text{thermal conductivity}, T = \text{Temperature},$$

$$Q = \text{interfacial heat transfer}$$

3.2. Geometry: -

- Column Geometry: Rectangular column with an aspect ratio of 3:1
  - Dimensions: 1500 mm (length) × 500 mm (breadth)
- Sparger Position: Placed 150 mm from one edge
- The column is filled with water upto 1.275m height.
- 83.3 percent of the column is filled with water.

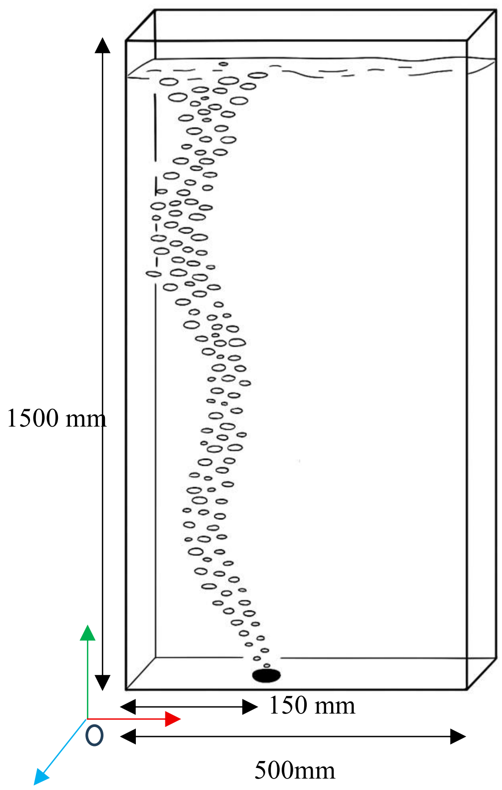

Figure 2: Geometry of the rectangular Bubble Column [2]

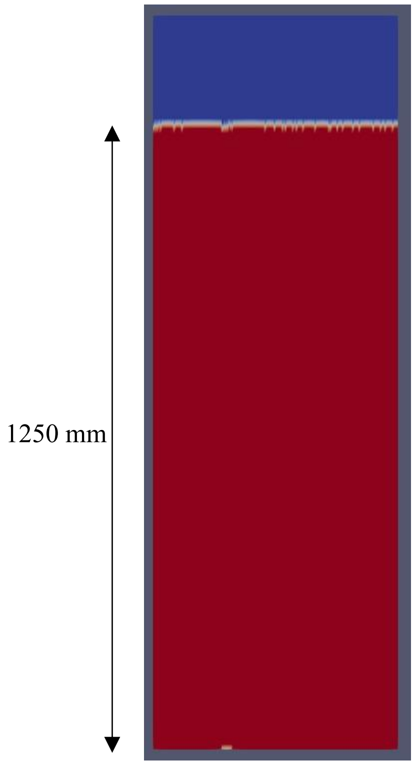

Figure 3: Volume Fraction of Air and Water

4. Simulation Procedure: -

4.1. Different Phases

Phase	Substance	Density ρ ($Kg*m^{-1}$)	Dynamic Viscosity μ (Pa*s)	Bubble Diameter d_p (m)	Surface Tension σ ($N*m^{-1}$)
Liquid	Tap water	$1 X 10^{3}$	$1 X 10^{-3}$	-----	$7.28 X 10^{-2}$
Gas	Air	1.2	$1.72 X 10^{-5}$	$4 X 10^{-3}$	-----

Table 1: Phases used in this simulation

4.2. Meshing

- The Mesh is structured mesh. The cells are uniformly distributed in y-direction.
- There is a local refinement near the inlet and outlet to better capture the Gas-Liquid interactions and bubble rise. The rest of the domain uses the coarser spacing for the mesh to maintain the computational efficiency.

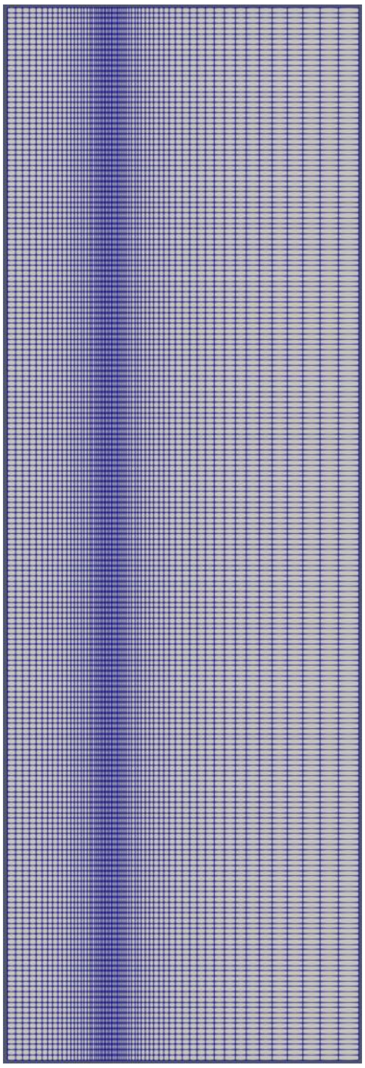

Figure 4: Meshing

|4.3. Boundary Conditions: -

Patch name	Inlet	Outlet	Walls
Alpha (air)	Uniform	zerogradient	zerogradient
Alpha (water)	Uniform	zerogradient	zerogradient
U (air)	fixedValue	zerogradient	noSlip
U (water)	fixedValue	zerogradient	noSlip

Table 2: Boundary Conditions

zeroGradient – It is the boundary condition that basically states that the value normal to the patch remains constant. That is the value is constant with respect to space.

fixed Value - It is the boundary condition that gives fixed value properties to each of the patches. In this boundary condition the value remains constant with respect to time

Uniform - It the boundary condition that has the same value at all the points on that boundary.

noSlip - It is the velocity boundary condition that enforces zero velocity at the walls. This boundary condition is based on the physical behaviour of the viscous flows.

4.4. Solvers: -

In OpenFOAM there are multiple solvers available to simulate the multiphase flow. Few Solvers are listed below:

Solvers	Approach	Compressibility	Flow Type	Fluid Type
cavitatingFoam	Homogeneous Equilibrium Model (HEM)	Incompressible	Laminar and Turbulent	Newtonian and Non-Newtonian Fluid
IncompressibleInterFoam	Volume of Fluid (VoF) approach	Compressible	Laminar and Turbulent	Newtonian and Non-Newtonian Fluid
driftFluxFoam	mixture approach with a drift-flux approximation	Incompressible	Laminar and Turbulent	Newtonian and Non-Newtonian Fluid
interFoam	Volume of Fluid (VoF) approach	Incompressible	Laminar and Turbulent	Newtonian and Non-Newtonian Fluid
interMixingFoam	Volume of Fluid (VoF) approach	Incompressible	Laminar and Turbulent	Newtonian and Non-Newtonian Fluid
interPhaseChangeFoam	Volume of Fluid (VoF) approach	Incompressible	Laminar and Turbulent	Newtonian and Non-Newtonian Fluid
multiphaseEulerFoam	Eulerian-Eulerian approach,	Incompressible	Laminar and Turbulent	Newtonian
twoPhaseEulerFoam	Eulerian-Eulerian approach,	Compressible	Laminar and Turbulent	Newtonian and Non-Newtonian Fluid

Table 3: Solvers list

Initially the multiphaseEulerFoam has been selected. But later, the solver has been changed to twoPhaseEulerFoam as there have been difficulties faced as it is comparatively easier and also ideal for the **dispersed – continuous** phase interactions.

The "**twoPhaseEulerFoam**" solver have following advantages:

- Both the phases are treated as interpenetrating continua, which is ideal for dense multiphase flow.
- This solver is suitable for bubble columns and fluidized beds.

- This also includes heat transfer and also multiple interfacial force models like drag, lift, wall lubrication, turbulent dispersion, etc.

4.5. Drag Model: -

The Drag model used in this Simulation is Schiller-Naumann. This drag model is widely used for simulating drag forces between fluid phases in multiphase flow. This model estimates the resistance caused by the relative motion between the particle and the surrounding fluid, in this case air bubble and water.

Applications of this model:

- Well suitable for situations involving spherical particles or bubbles, where the deformation is negligible.
- Low Void fraction.
- Best suitable for simulating particle-fluid interactions.

Limitations of this model:

- This model is not suitable for highly deformed particles.
- It is not applicable for high void fractions.
- It is not applicable for high Reynold number.
- This model's performance reduces in non-isothermal conditions.

The drag function is given as: - $f = \frac{(C_D * Re)}{24}$ (5)

The Drag Coefficient, $C_D = \begin{cases} \frac{24(1+Re^{0.687})}{Re}, & Re \leq 1000 \\ 0.44, & Re \geq 1000 \end{cases}$ (6)

The relative Reynold number (Re) for the primary phase and secondary phase represented as p and q respectively is given as: -

$$Re_{pq} = \frac{\rho_q |\vec{v_p} - \vec{v_q}| d_p}{\mu_q} \quad (7)$$

The relative Reynold number (Re) for the secondary phases p and r respectively is given as: -

$$Re_{rp} = \frac{\rho_{rp} |\vec{v_r} - \vec{v_q}| d_{rp}}{\mu_{rp}} \quad (8)$$

5. Results: -

5.1. Velocity Vs Height of Column:

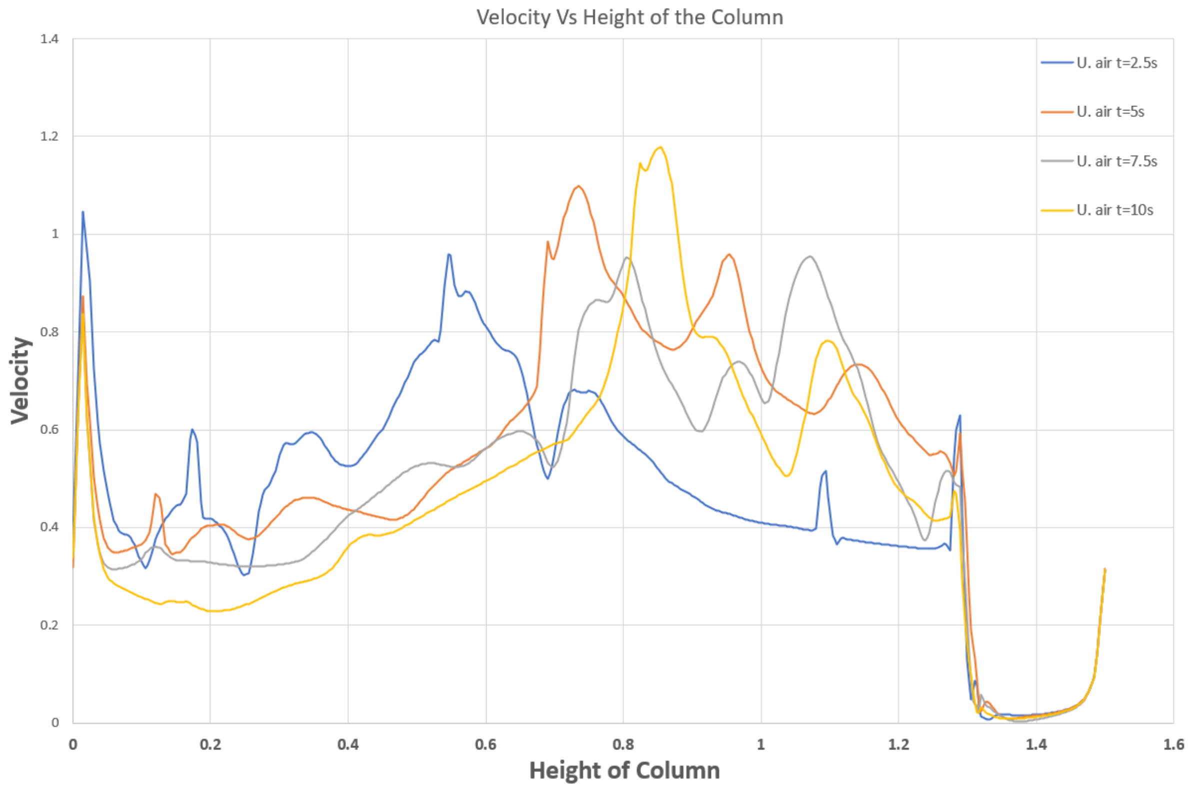

Figure 5: Velocity vs Height of Column for U=0.2m/s at x=0.15m

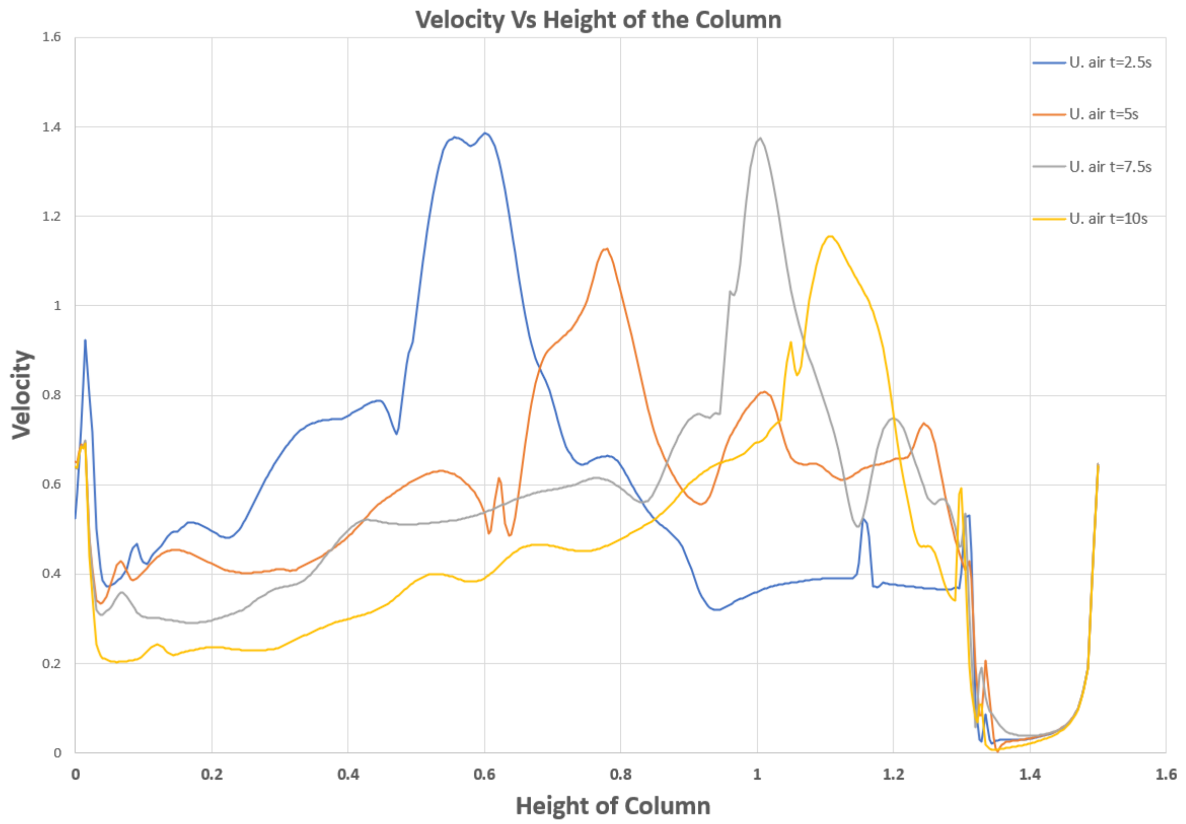

Figure 6: Velocity vs Height of Column for U=0.4m/s at x=0.15m

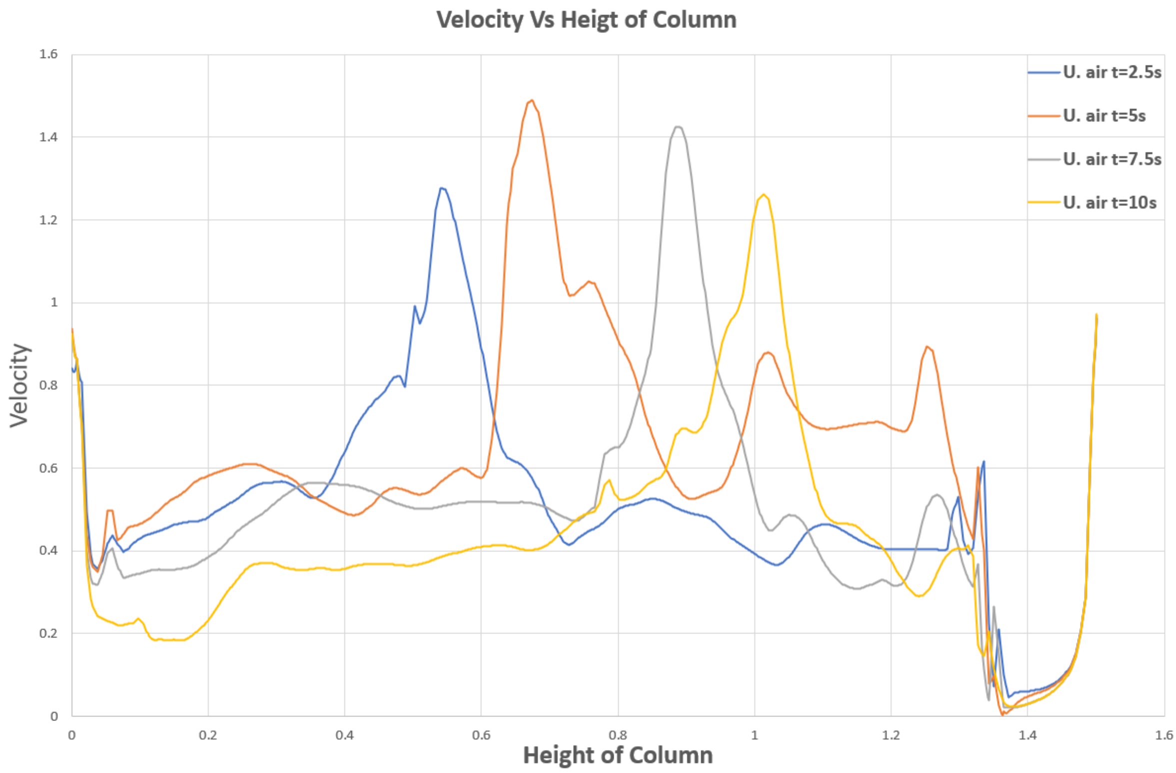

Figure 7: Velocity vs Height of Column for U=0.6m/s at x=0.15m

These Plots describe about the velocity at different heights of the column. They are plotted at x=0.15 from origin in which the axis passes through the inlet and the outlet.

- It can be seen that there is peak in velocity near the inlet where air is being injected at all the three different velocities.
- Near the inlet the bubble diameter is small and they have high relative velocity compared to the fluid in the column and this might lead to the following:
  - Large drag forces
  - High terminal velocities
  - Strong momentum exchange
- As the air flows upwards, the mixing or the fluctuations increase to a certain height and dies due to energy dissipation and bubble coalescence.
- The peaks and drops describe the turbulent nature of the air-liquid nature which in turn causes the vortex formation and bubble plume behaviour.
- Over time the velocity of the air falls especially near the middle and top zones which shows the momentum loss.
- As the air flows up, they combine and form bigger bubbles which face. The opposing buoyancy dominates the drag on the bubble hence accelerating the bubble, which can be seen in the above graphs.
- The peak velocity is at certain height of column and not at the inlet. After certain amount of the time, the bubbles combine to form bigger ones in which the buoyancy force acting on it increases resulting in acceleration of the bubble.

The figures mentioned below show the velocity of the air flow at different time steps for U=0.6m/s.

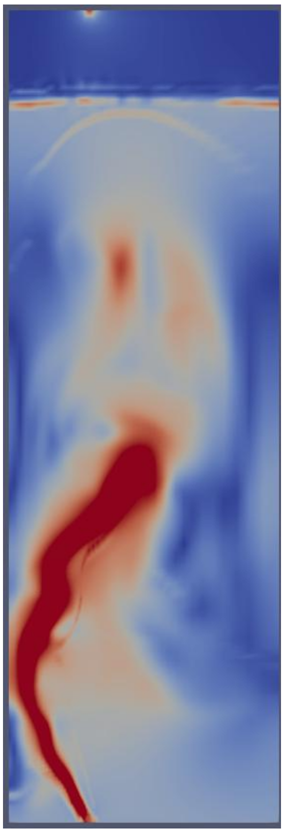

Figure 8: at t = 2.5s

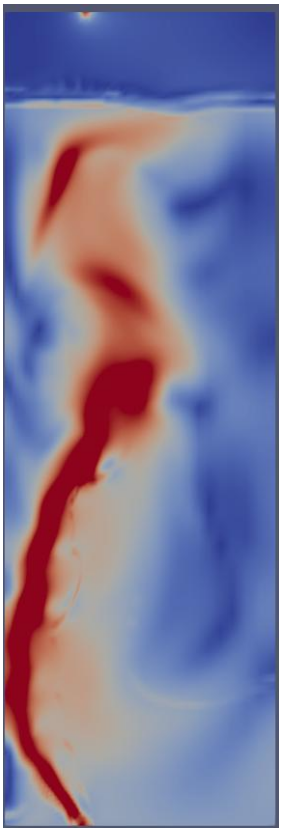

Figure 9: at t = 5s

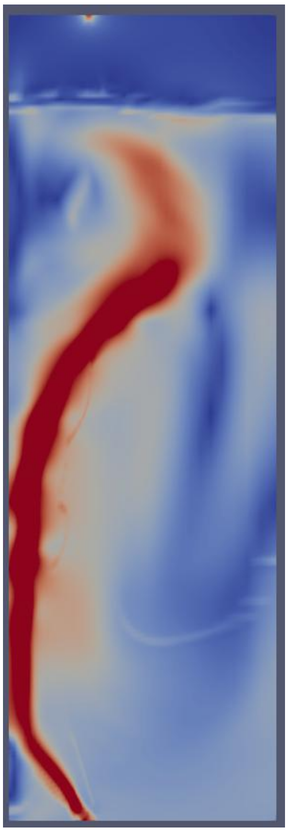

Figure 10: at t = 7.5s

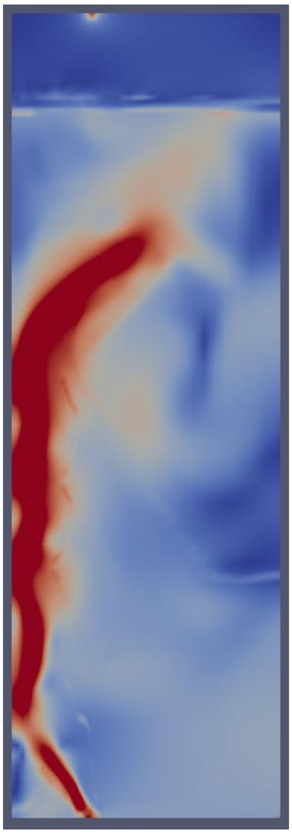

Figure 11: at t = 10s

5.2. Voidage Vs Width of Column:

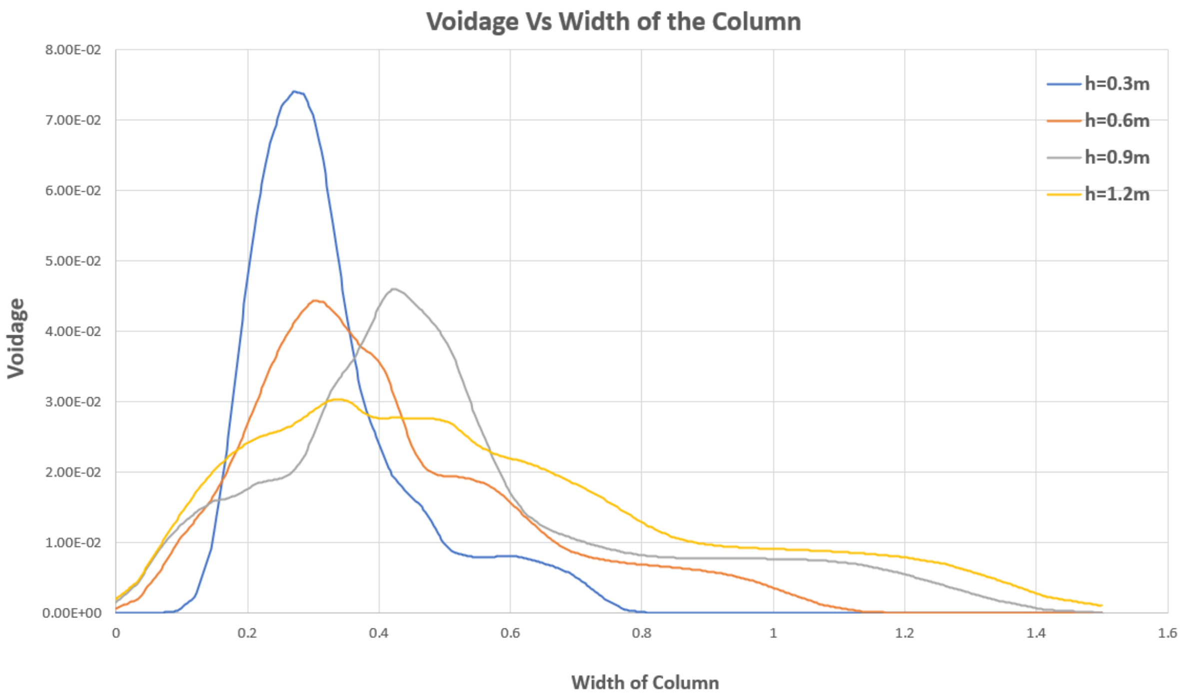

Figure 12: Voidage Vs Width of Column at t=5sec for U=0.2m/s

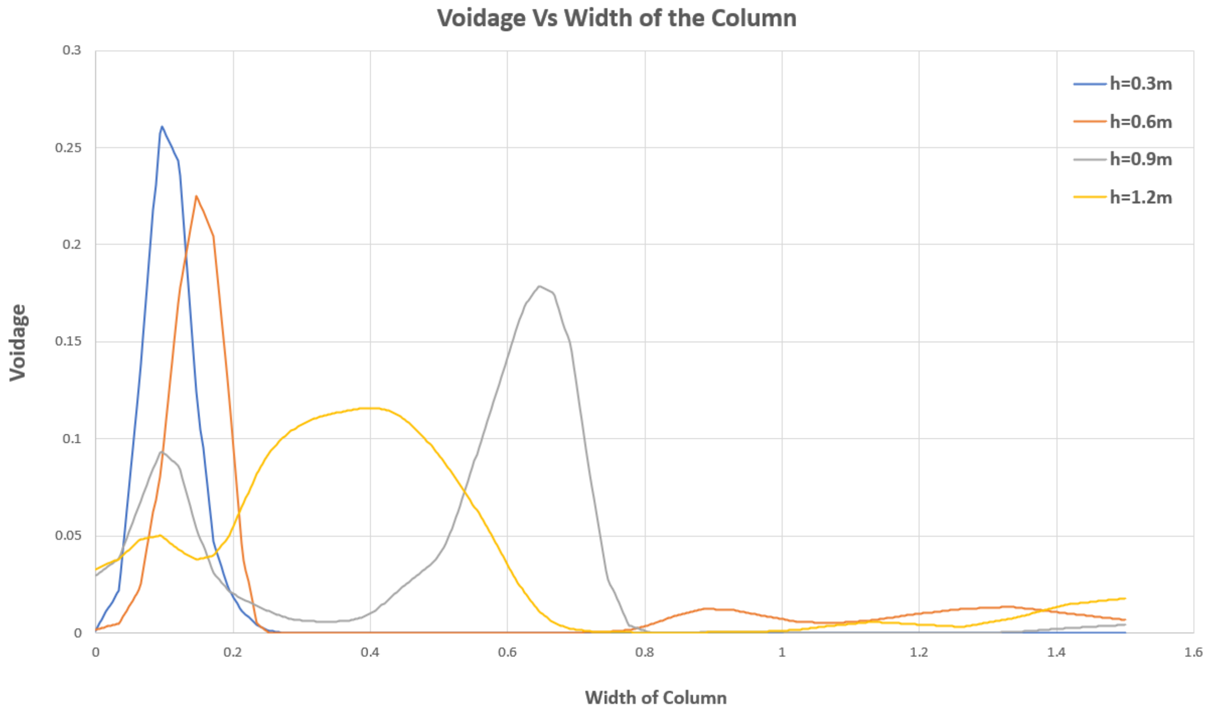

Figure 13: Voidage Vs Width of Column at t=5sec for U=0.4m/s

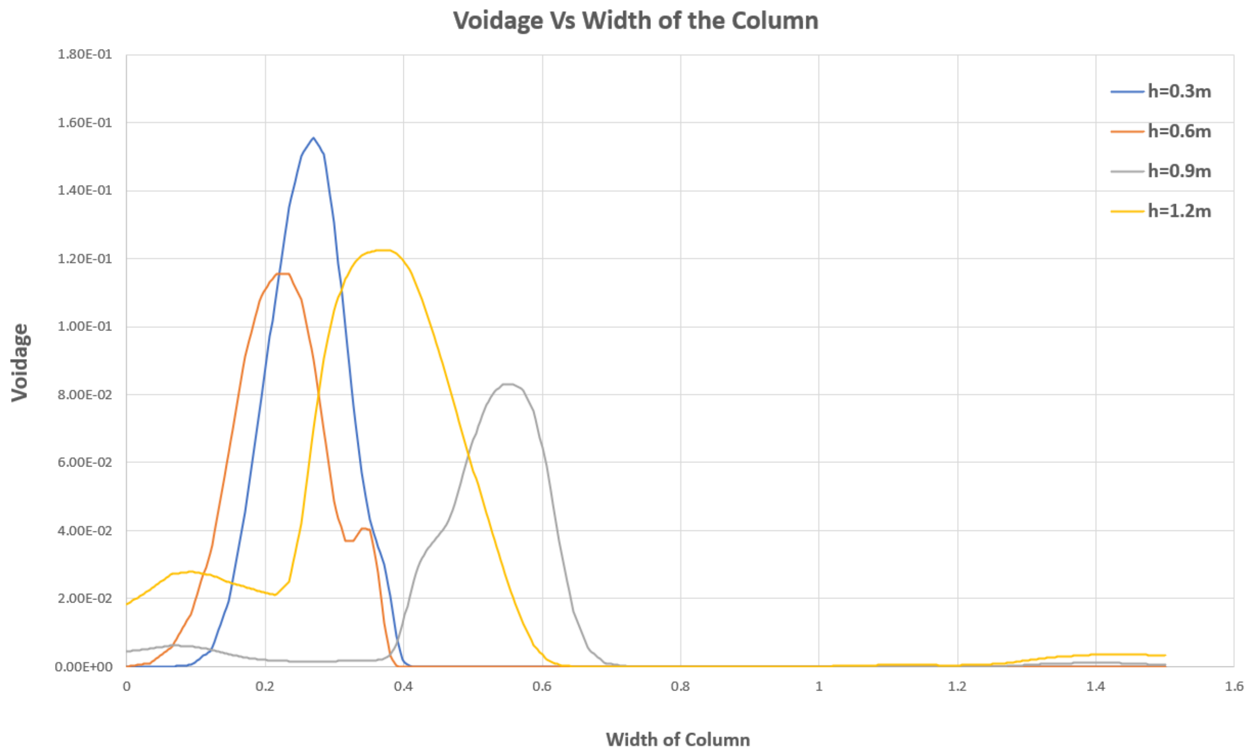

Figure 14: Voidage Vs Width of Column at t=5sec for U=0.6m/s

The above-mentioned plots describe the void fraction of air i.e., the volume fraction occupied by the air in that location along the width of the column at t=5sec.

- It can be observed that there is sharp peak near the inlet, this indicates high concentration of air near the inlet, which is due to injection of air.
- The shifts in peaks indicate the spread of the bubbles. Air void fraction decreases because of dispersion and mixing of the air with the liquid in the column. As we go along the height of the column, due to turbulent diffusion and wake interactions, the bubbles in the water get dispersed laterally.

The figures below show the void fraction of the air for different inlet velocities at t=5 sec.

Figure 15: U=0.2 m/s

Figure 16: U=0.4 m/s

Figure 17: U=0.6 m/s

5.3. Pressure Vs Time:

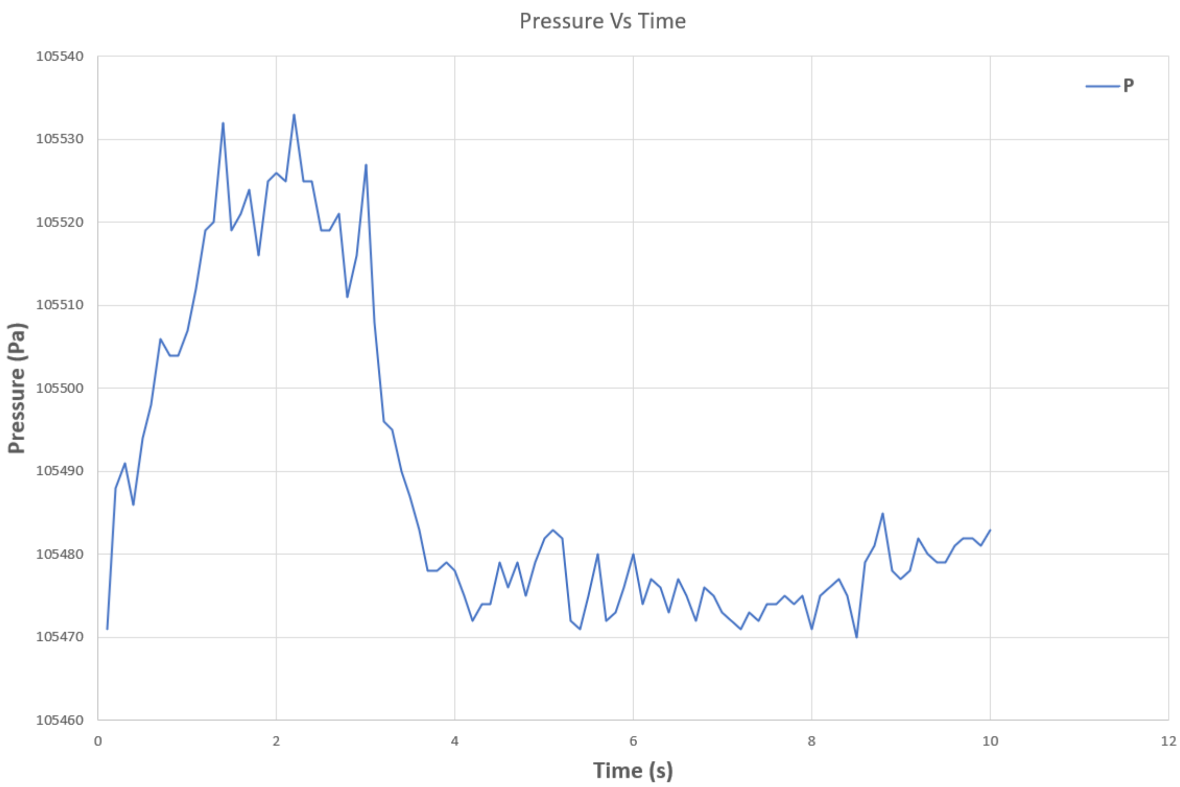

Figure 18: Average Pressure Vs Time for inlet velocity U=0.2m/s

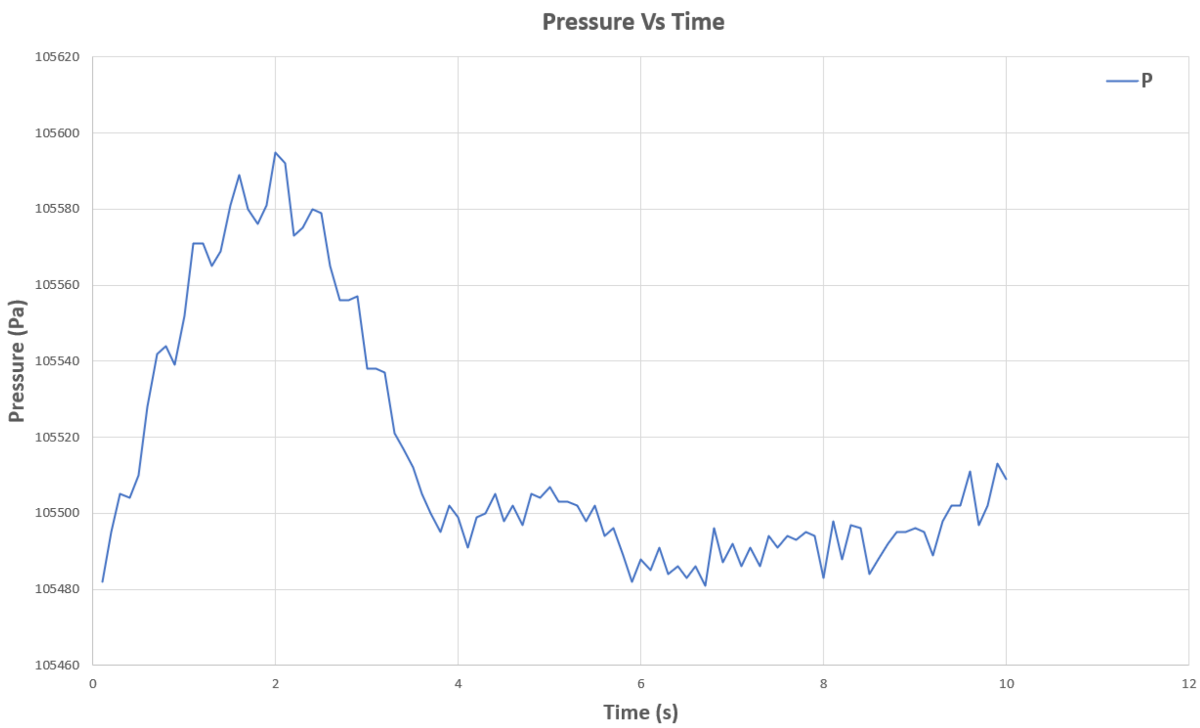

Figure 19: Average Pressure Vs Time for inlet velocity U=0.4m/s

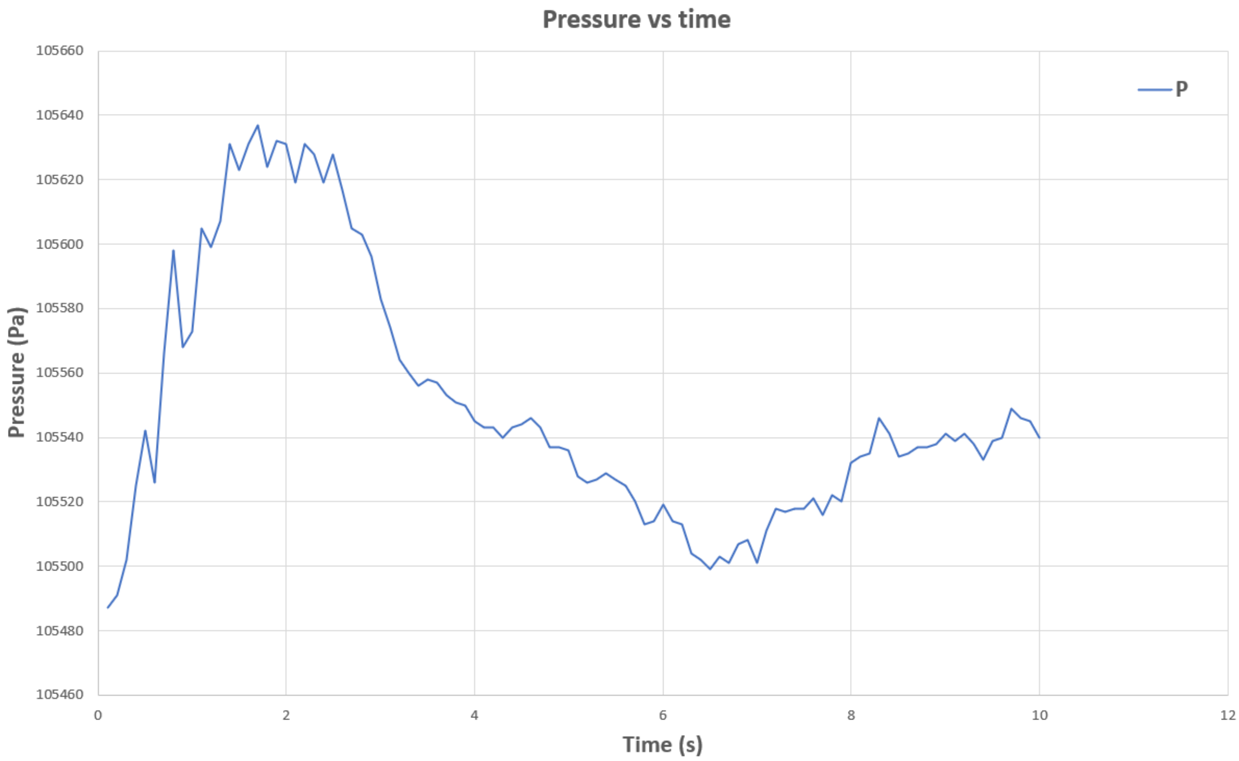

Figure 20: Average Pressure Vs Time for inlet velocity U=0.6m/s

In graphs mentioned above are the average Pressure Vs the total time of the Bubble Column for all the different velocities.

- This pressure and the fluctuations gradually decrease after certain amount of time.
- There are low amplitude fluctuations in the Pressure which are caused by the following:
  - Bubble Coalescence
  - Breaking of the bubbles.
- As the bubbles rise up, they create transient pressure waves in the liquid, which is caused due to varying local void fractions.
- The major causes of Pressure fluctuations are:
  - Unsteady injection of air into the Bubble Column.
  - Combining and separation of Bubbles.
  - Slug or Churn flow formation in the Bubble Column.
  - Turbulence and Vortices formation.

6. Challenges: -

- Assigning the wrong Boundary conditions initially.
- Could not initialize the water air ratio in the column.
- Could not enable the drag model which has been used.

- Faced issues to maintain the courant number < 1, initially.
- The temperature values were unrealistic.

7. Conclusion: -

In the present study, numerical simulations have been carried out using the open source CFD software OpenFOAM to simulate "*Simulation of gas-liquid bubble column contactor*". OpenFOAM solver "twoPhaseEulerFoam" has been used in simulations. Detailed step-by-step procedure, boundary conditions, initial conditions as well as solver details are explained in the report. The device used for the study is an Intel i5 12th gen 64-bit processor, 16 Gb RAM, Ubuntu 22.04 LTS on OpenFOAM version 7.

8. Future Work: -

1. Simulate the Bubble Column case with high inlet velocity and also increase the time of the simulation.
2. Simulate the case for various Turbulence models.
3. Convert this 2D model case into 3D model and simulate it.

9. Tips for Simulating Gas-Liquid Two Phase Flow

- Usage of fine Mesh near the inlet and outlet for accurate results.
- To initialize the setFieldsdict file before the start to simulation.
- To assign proper Boundary conditions.
- Choosing the right turbulence model based on the requirement.
- Enabling the adaptive time step to maintain the courant number (<1).
- Monitor the residuals, Courant number and time step size during the simulation.

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