Implementation of custom drag model in a bubble column reactor

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Abstract

In biotechnological and chemical technology fields there are various applications of bubble column reactor which is significant from other equipment. At the basics the bubble column is a structure in which water is filled inside and gas is passed through it from the bottom. The behaviour of gas bubbles greatly affects the efficiency of these processes. This research uses a custom drag force model which is based on the Ishii Zuber drag force model to test the air phase volume fraction in a bubble column domain. The setup includes a bubble column which is of the cylindrical domain where the gas phase is injected into the liquid with the help of a sparger at a superficial gas velocity of 10 cm/s. The multiphase CFD model is created using OpenFOAM v7, a free and open-source software, to analyse the flow interaction between the gas-liquid phase system. The study looks at the different height in the bubble column and the time averaged Air phase volume fraction is found at all locations to study the spread of air molecules within the column, and the end analysis results had been compared with existing liable experimental data from the research papers based on the bubble column literatures.

KEYWORDS: OpenFOAM, CFD, Bubble Column, Multiphase

1. Introduction

The study of gas-liquid hydrodynamics is essential for many industrial and biotechnological applications as the behaviour of gas bubbles in a liquid medium needs to be controlled with remarkable precision so that it can meet quite constitute particles. In Chemical Reactors, bioreactors and other multiphase systems usually gas is sparged at the bottom of the reactor to help in mixing and driving specific chemical reactions. Behaviour of these processes is mainly related to solution bubble gas dynamics as the latter affects the flow field and consequently mixing inside a column.

One aspect of the study gas-liquid interactions are important to optimize reactor design and operation, especially in systems like bubble columns that are extensively used industrially for processes such as wastewater treatment, fermentation or chemical synthesis. One of these powerful tools is Computational Fluid Dynamics (CFD) that have been proven useful for the simulation of such multimodal and multiscale systems to analyse in detail some hydrodynamic features which sometimes are difficult or quite impractical to measure by a traditional experimental setup. OpenFOAM includes a suite of advanced multiphase flow models, which can be customized for different applications, making it an attractive tool to simulate phenomena in complex systems such as gas-liquid bubble columns. This study aims to investigate the effect of the new drag force model and study the air volume fraction within the bubble column reactor.

2. Problem Statement

The key objective of this study is to study the Volume fraction of air in the bubble column reactor with a custom drag force model through computational modelling of Multiphase flows. To implement the CFD model a 3D bubble column reactor is selected for the computational domain, (figure 1).

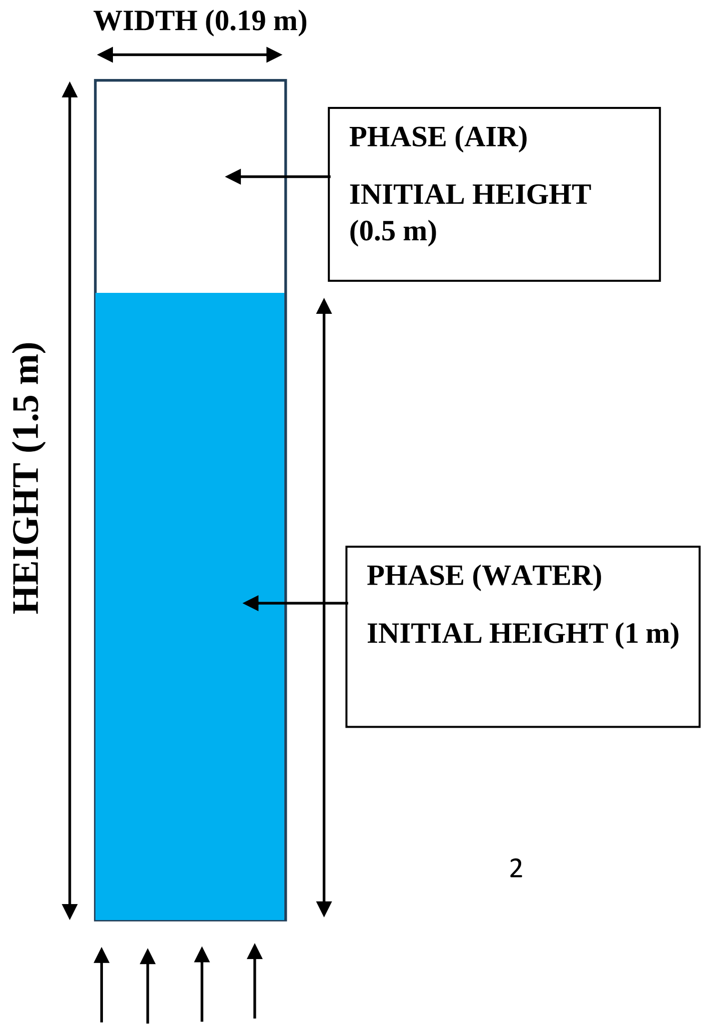


Figure 1: Bubble Column dimensions and initial Volume fractions

3. Governing Equations

Model simplifications were implemented, including the assumption of isothermal conditions and density of phase Air that is either fixed value or varies with in system pressure as defined by the proven ideal gas law equation. These Equations that governing fluid gas flow interactions are as follows:

3.1 Continuity equation:

$$\partial/\partial t\,(\alpha_a\,\rho_a) + \nabla.\,(\alpha_a\,\rho_a\,\overrightarrow{u_a}) = 0 \qquad (1)$$

In this context, 'a' represents the phases, which can be either gas or liquid. The symbol ρ_a indicates the mass by volume of the phase 'a', while α_a refers to percent of phase present within the system (Void fraction of phase). Additionally $\overrightarrow{u_a}$ signifies the rate of speed that the phase is sent into the system.

3.2 Momentum equation:

$$\partial/\partial t\,(\alpha_a\,\rho_a\,\overrightarrow{u_a}, i) + \overrightarrow{u_j}\,\partial/\partial x_j\,(\alpha_a\,\rho_a\,\overrightarrow{u_a}, i) = -\alpha_a\,\partial P/\partial x_i$$

$$+\ \partial/\partial x_j\ \ (\alpha_a\,(\mu_a+\mu_a, t)\,\partial\overrightarrow{u_{a_i}}/\partial x_j) + \alpha_a\,\rho_a\,\vec{g} + Fa \qquad (2)$$

In this context, $\vec{g}$ represents the rate of velocity to force of gravitation, μ_a signifies the viscosity of the phases that is interacted within the system ‘a’, μ_a, t indicates the fluid turbulence action viscosity property of phase ‘a’, Fa refers to the terms which may encompass force due to lift action, turbulence action of fluid dispersion force, induced drag force, and virtual force due to the relative motion of the molecules of the phases.

3.3 Mixture k–ε model:

Mixture k-epsilon turbulence model is employed due to, at elevated phase volume fractions of Air and Water within the domain of consideration that behave as one cohesive unit, necessitating the resolution of turbulence equations for the mixture. A significant feature of this model is that it requires the solution of only a single set of velocity components, which greatly diminishes the effort of solving. The k – ε system equations that are utilized to describe the system.

$$\frac{\partial}{\partial t}(\rho_m k) + \nabla.(\rho_m \overrightarrow{v_m} k) = \nabla.\left(\frac{\mu_{t,m}}{\sigma_k}\nabla k\right) + G_{k,m} - \rho_m \varepsilon \qquad (3)$$

$$\frac{\partial}{\partial t}(\rho_m \varepsilon) + \nabla.(\rho_m \overrightarrow{v_m} \varepsilon) = \nabla.\left(\frac{\mu_{t,m}}{\sigma_\varepsilon}\nabla \varepsilon\right) + \frac{\varepsilon}{k}(C_{1\varepsilon} G_{k,m} - C_{2\varepsilon}\rho_m \varepsilon) \qquad (4)$$

The generation of the energy of kinetic source term Gk,m is expressed as follows:

$$G_{k,m} = \mu_{t,m}(\nabla \overrightarrow{v_m} + (\nabla \overrightarrow{v_m})^T) \qquad (5)$$

Where turbulent viscosity μt, miscomputed from,

$$\mu_{t,m} = \rho_m C_\mu \frac{k^2}{\varepsilon} \qquad (6)$$

The calculation of the mixture of air and water phase density (ρm) and mixture of air and water phase velocity is performed as follows:

$$\rho_m = \sum_{i=1}^{2} \alpha_i \rho_i \qquad (7)$$

$$\overrightarrow{v_m} = \frac{\sum_{i=1}^{2} \alpha_i \rho_i \overrightarrow{v_i}}{\sum_{i=1}^{2} \alpha_i \rho_i} \qquad (8)$$

Cμ is a model constant of the integration. The current value of this model constant is 0.09.

3.4 Bubble drag force:

Drag force originates due to pressure differences and frictional forces between the phases and acts in the opposite direction to the movement. Various drag models are available like Schiller Naumann, Tomiyama correlated, Tomiyama analytical, Ishii Zuber etc. [7][8][10]. Drag forces are given by,

$$F_{drag} = -\frac{3}{4d_B} C_D \rho_l \alpha_g |\overrightarrow{v_g} - \overrightarrow{v_l}|(\overrightarrow{v_g} - \overrightarrow{v_l}) \qquad (9)$$

Here d denoted the bubble diameter of the air bubble. The drag coefficient, denoted as Cd, is influenced by the flow regimes, which are determined by the Reynolds number, as well as the characteristics of the continuous phase, including density and viscosity. It is important to note that the drag coefficient for an individual bubble differs from the drag forces experienced in a bubble column. The calculation of the drag coefficient for a solitary bubble ascending in a liquid is performed as follows.

$$C_{Do} = \max(C_{D,sphere}, \min(C_{D,ellipse}, C_{D,cap})), \qquad (10)$$

For the Ishii Zuber drag model the following were the correlations,[8]

$$C_{D,sphere} = \frac{24}{Re}(1 + 0.1Re^{0.75}), \qquad (11)$$

$$C_{D,ellipse} = \frac{2}{3}\sqrt{Eo}, \qquad (12)$$

$$C_{D,cap} = \frac{8}{3} \qquad (13)$$

The influence of bubbles on the drag coefficient associated with an individual bubble. Modification was made in the Ishii Zuber model, and a correction term was introduced [1],

$$f(\alpha_g) = (1 - \alpha_g)^p \qquad (14)$$

Here f (α_g) is the correction term and is multiplied by the drag coefficient. The parameter p is assigned a value of 2 when the superficial gas velocities are low, specifically below 20 cm/s, and a value of 4 when the superficial gas velocities are high, ranging from 20 to 40 cm/s. [1]. The steps to implement the custom drag model in OpenFOAM is given in the appendix for more brief explanations.

The equations that are responsible for the simulation were addressed in transient work conditions utilizing the CFD solver OPENFOAM v7, specifically the twophaseEulerFoam solver is used as there are two phases involved within the simulation. In the simulations air is considered as the dispersed fluid phase and the continuous fluid phase is considered as water. Accounting for turbulence in the gas phase, mixture k-epsilon turbulence model was applied. In the twophaseEulerFoam solver, the fundamental Ishii Zuber model was modified based on equations (14) to incorporate the neighbouring effects of bubbles, which were implemented through coding and compilation within the solver. It was generally observed that the virtual mass force was negligible in comparison to the other concerning forces like drag and lift forces; hence, it was excluded from consideration. Although the lift force was found to be less than the drag force, its formulation was deemed necessary as it influences the radial distribution of gas hold-up. An optimal bubble size of 3 mm has been reported, and consequently, a constant bubble size of 3 mm was utilized in all simulations.

4. Simulation Procedure

4.1 Geometry and Mesh

The column has a Radius (R) of 9.5 cm and a total length (H) of 150 cm, as indicated in reference [1]. Water was introduced to a height of 100 cm. Phase air was introduced in the outlet and distributed across the secctional area of the column. The three-dimensional geometry was developed using ICEM ansys CFD software. The Mesh generated consisted of 116,369 cells. The maximum aspect ratio recorded was 4.5786, while the maximum skewness was noted at 0.79. The orthogonality of the mesh was measured at 29.7, which is below the threshold of 30. The bottom face of the cylinder serves as the inlet, whereas the top face functions as the outlet, with the surrounding structure consisting of walls. To accurately find the change in flow variables adjacent to the wall an O-grid type of special mesh was implemented in that region. Hexahedral type of mesh structure was used to generate the domain. Figure 5, representation of the computational domain.

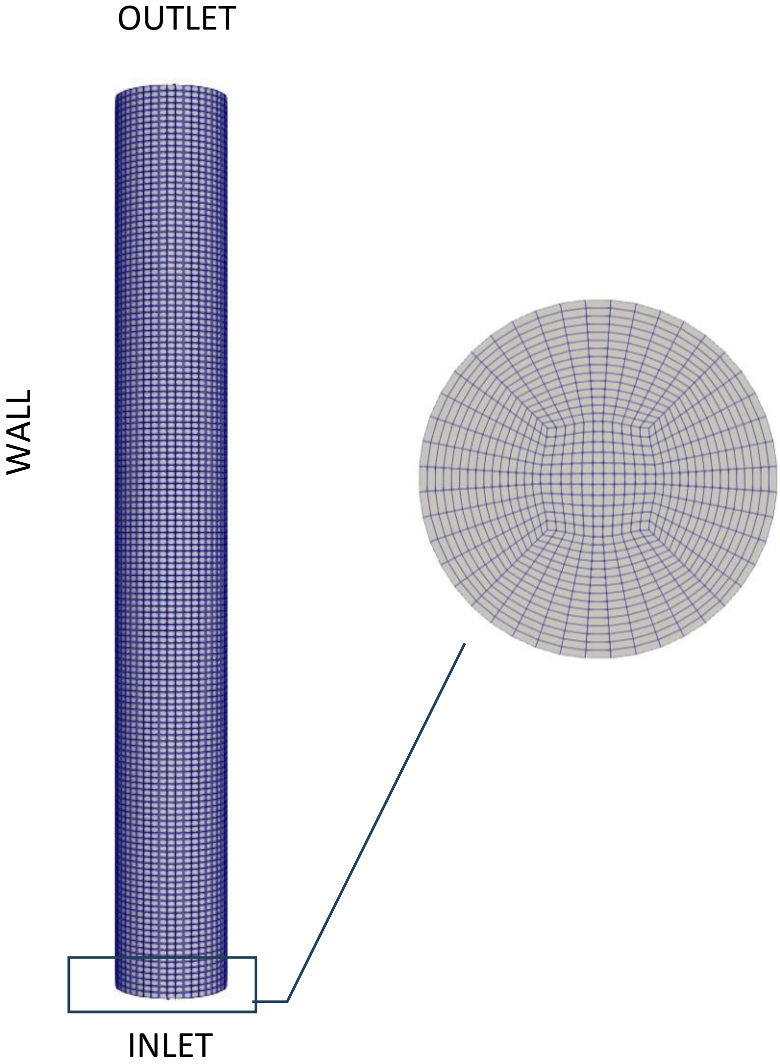


Figure 5: Top view and side view of the bubble column domain the cells of 116369 cells

4.2 Initial and System Boundary Conditions

INLET FLOW BOUNDARY CONDITION:

At inlet the volume fraction of Air is set to a value of 1 which also gives a meaning that it is fully porous, and the air is uniformly distributed at the inlet. The pressure is given a constant value of atmospheric value that is 1e5. The velocity of the Phase air is used as 0.1 m/s which makes the air molecules to flow within the system of fluid. The water velocity is set to 0 to prevent flow of water out the system.

INLET	TYPE	VALUE
Alpha. air	*fixedValue*	*1*
Pressure	*fixedFluxPressure*	*1e5*
Air velocity	*fixedValue*	*0.1 m/s*
Water velocity	*fixedValue*	*0 m/s*

Table 1: inlet boundary conditions.

OUTLET FLOW BOUNDARY CONDITION:

At outlet the volume fraction of air is set to 1 and the special condition of inlet outlet condition in which the value is set to 1 for normal flow direction and for opposite flow the condition changes to zero gradient. The pressure is given by prgh pressure condition and set to atmospheric condition. The velocity of phase air is given a condition as pressure inlet outlet velocity which manages the flow characteristics at outlet. Same for water and it is ensured that water doesn’t flow out of the system.

OUTLET	TYPE	VALUE
Alpha. air	*inletOutlet*	*1*
Pressure	*prghPressure*	*1e5*
Air velocity	*pressureInletOutletVelocity*	-
Water velocity	*pressureInletOutletVelocity*	-

Table 2: outlet boundary conditions.

WALL BOUNDARY CONDITION:

At wall the flow condition for volume fraction is set to a fixed value of zero, which means that the value of air void fraction in the wall elements doesn't change and is fixed as zero. For velocity components of air and water it is set to zero in all directional components. Additionally, a fixedFluxPressure boundary condition is implemented at the wall for pressure.

WALL	TYPE	VALUE
Alpha. air	*fixedValue*	*0*
Pressure	*fixedFluxPressure*	*1e5*
Air velocity	*fixedValue*	*(0, 0, 0)*
Water velocity	*fixedValue*	*(0, 0, 0)*

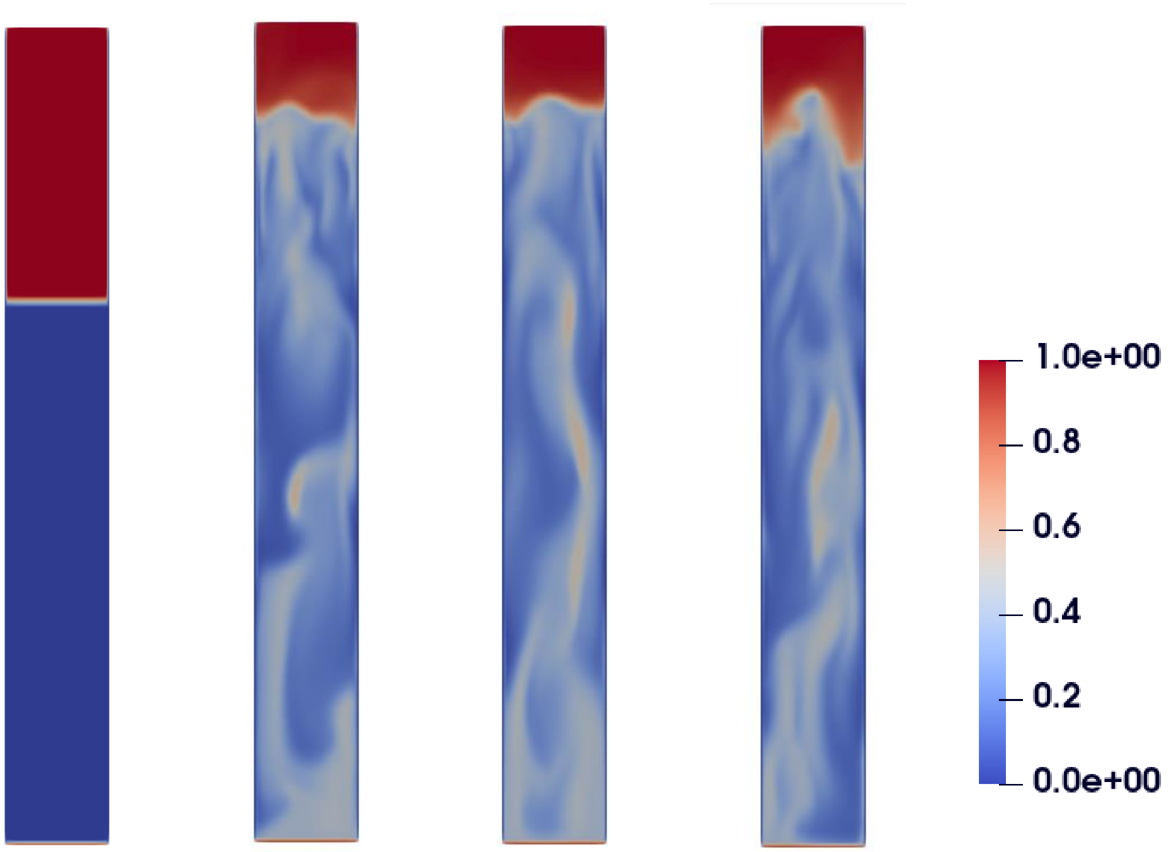
Table 3: wall boundary conditions.

4.3 Solver

twoPhaseEulerFoam serves as a solver designed for a system comprising two non-reacting compressible fluid phases. In this configuration, one of the phases is consistently dispersed, making it particularly suitable for the simulation of bubble columns in gas-liquid systems, as well as fluidized and spouted beds in gas-solid systems. For gas-liquid interactions, users can choose from various laminar and turbulence models, including RAS and LES, applicable to both phases. Additionally, the solver offers a range of sub-models for interphase coupling, allowing for the selection of diverse physical models tailored to the system. Furthermore, users have the capability to enhance the standard solver by incorporating new sub-models into their simulations.

5. Results and Discussions:

Post-processing of the results was carried out in Paraview and Excel for the Results obtained. The results were computed to 150 seconds with the last 50 seconds averaging the Volume fraction of Air to get the Time averaged Volume fraction of air. Volume fractions in different locations were calculated and plotted over the diameter of the bubble column.



At T = 0 seconds At T = 10 seconds At T = 20 seconds At T = 150 seconds

Figure 6: Volume fraction of Air at different time steps concerning X plane for velocity of 0.1 m/s of Air.

The time-averaged volume fraction of air is shown in Figure 7. The average volume fraction of air is shown for the location of 0.225 m from the inlet of the bubble column.

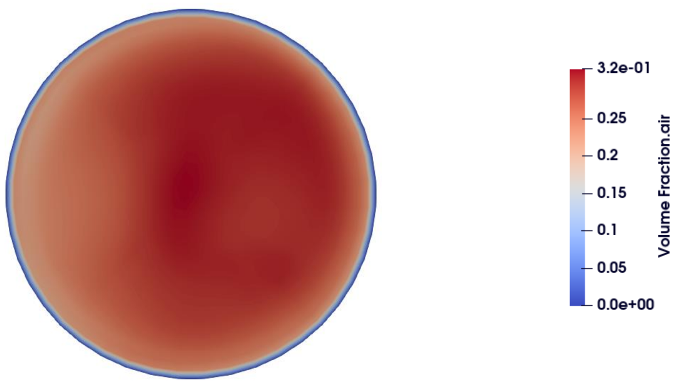


Figure 7: Averaged Volume fraction (0.225m) in Z normal

From this, the time-averaged plot is plotted for the volume fraction of Air at different locations (0.225 m, 0.825 m) using the average of 15 different line plots in different locations.

5.1: Time Averaged Volume Fraction of air at 0.225 m:

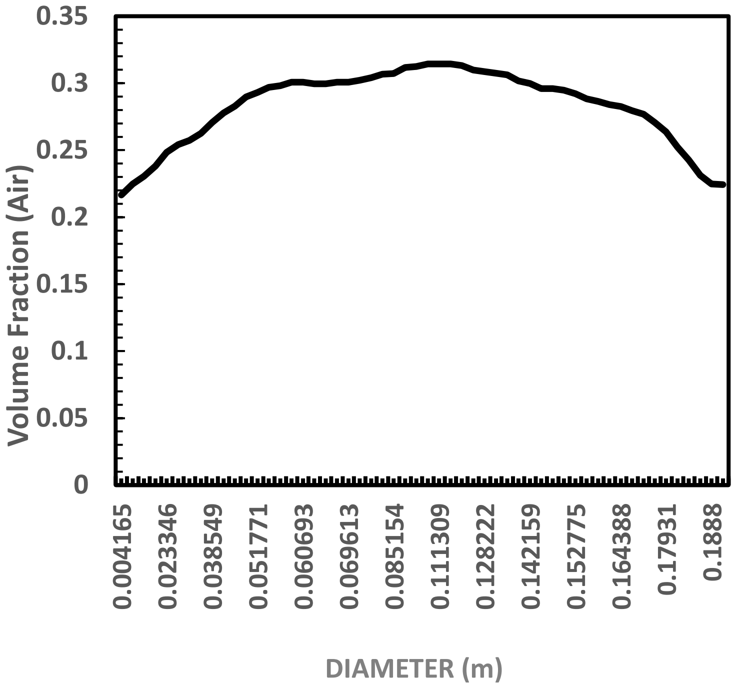


Figure 8: Average Volume fraction of air at 0.225 m

From Figure 8, we can infer that the maximum volume fraction value is 0.32 which is located at the middle of the bubble column reactor 0.095 m for the velocity of 0.1 m/s.

5.2: Time Averaged Volume Fraction of air at 0.825 m:

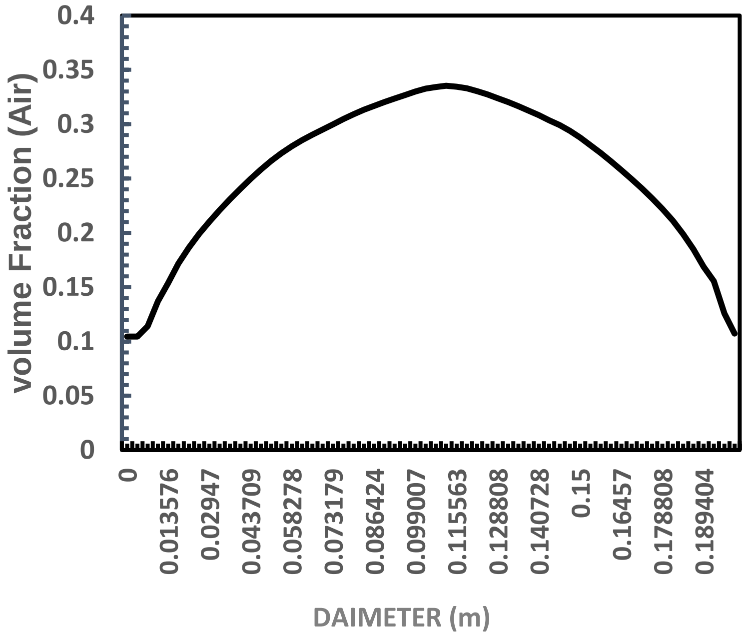


Figure 10:Average Volume fraction of air at 0.825 m

From Figure 10, we can infer that the maximum value of the volume fraction is 0.33 at the location of 0.11 m in the diameter of the bubble column. In the wall, the value starts from 0.1 and increases gradually in the parabolic curve. Thus, the modification proposed in [1] is used for the Ishii Zuber drag model and the results are obtained.

6. CONCLUSION:

In the current investigation, a new drag force model addressing the volume fraction of air in a two-phase bubble column is thoroughly examined utilizing the open-source computational fluid dynamics software OpenFOAM v7. The primary contribution of this research lies in the simulation of customized drag effects within a cylindrical bubble column reactor, referencing existing literature data for a superficial velocity of 10 cm/s to develop a suitable multiphase simulation model. At different heights in the column from the axial direction many plot were plotted to study the volume fraction of air values and distribution across the column diameter. The proposed model, multiphase simulation of bubble column was performed with the modifications that had been implemented to the Ishii Zuber drag force equations wherein the special term p is assigned a value of 2 for gas phase velocities that are less than of ≤20 cm/s and 4 for gas phase velocities that are between 20 cm/s to 40 cm/s. Additionally, the mixture k–ε turbulence model is recommended to effectively simulated the source force terms like drag force model and wall induced turbulence and turbulence due to moving of bubbles within the column. This study may be further expanded to include more detailed analysis of the source terms and implementing new turbulence and population balance models which ensures the mass balance within the bubble column which is important for many industrial applications.

References

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APPENDIX:

IMPLEMENTATION OF CUSTOM DRAG MODEL:

To implement custom drag model the required files, need to be modified and complied with the OpenFOAM.

- → Custom drag model .C file
- → Custom drag model .H file
- → Make Folder
    - ♦ Files
    - ♦ Options

In the .C file the back-end code which must be executed need to be updated and in .H file the dependencies for that custom drag model must be updated. (Figure 2)

In Make folder the files required for compilation are present, in files the path of library in which the custom drag model should be update is present. (Figure 3)

In options files the paths of dependencies that are required for the drag model to run are present. (figure 4).

(In every file the name of the drag model should be changed to the custom drag model name used)

.C file and the modified Ishii Zuber drag Model code:

```
// * * * * * * * * * * * * * * * * Member Functions  * * * * * * * * * * * * * * * //

Foam::tmp<Foam::volScalarField>
Foam::dragModels::IshiiZuberModv::CdRe() const
{
    volScalarField Eo(max(pair_.Eo(), scalar(1e-3)));
    volScalarField d(pair_.dispersed().d());
    volScalarField rho(pair_.continuous().rho());
    volScalarField magUr(pair_.magUr());
    volScalarField Re(max(pair_.Re(), scalar(1e-3)));
    volScalarField alpha1
    (
        max(pair_.dispersed(), pair_.dispersed().residualAlpha())
    );
    //scalarField p; // to get p value from user
    volScalarField correction (pow((1-alpha1), 2));
    volScalarField CdSphere (24.0 / Re * (1. + 0.15 * pow(Re,0.687)));
    volScalarField CdEllipse ((4.0/3.0) * pow(2. * Eo , 0.5));
    // volScalarField CdCap ((8.0/3.0));
    volScalarField Cd (max(CdSphere, min(CdEllipse, 2.666667)));
    return (Cd * correction) * Re ;
}
```

Figure 2: Modified code for Ishii Zuber Drag model.

Make folder > files:

```
IshiiZuberModv.C

LIB = $(FOAM_USER_LIBBIN)/libIshiiZuberModvModel
```

Figure 3: files context

Make folder > options:

```
EXE_INC = \
    -I$(LIB_SRC)/transportModels/lnInclude \
    -I$(LIB_SRC)/thermophysicalModels/basic/lnInclude \
    -I$(LIB_SRC)/finiteVolume/lnInclude \
    -I$(FOAM_SOLVERS)/multiphase/twoPhaseEulerFoam/interfacialModels/lnInclude \
    -I$(LIB_SRC)/finiteVolume/lnInclude \
    -I$(LIB_SRC)/meshTools/lnInclude \
    -I$(LIB_SRC)/transportModels/compressible/lnInclude \
    -I$(LIB_SRC)/thermophysicalModels/basic/lnInclude \
    -I$(LIB_SRC)/transportModels/incompressible/transportModel \
    -I$(LIB_SRC)/TurbulenceModels/turbulenceModels/lnInclude \
    -I$(LIB_SRC)/TurbulenceModels/compressible/lnInclude \
    -I$(LIB_SRC)/TurbulenceModels/phaseCompressible/lnInclude \
    -I$(FOAM_SOLVERS)/multiphase/twoPhaseEulerFoam/twoPhaseSystem/lnInclude

LIB_LIBS = \
    -lfiniteVolume \
    -lcompressibleTwoPhaseSystem \
    -lcompressibleTransportModels \
    -lfluidThermophysicalModels \
    -lspecie
```

Figure 4: option file context.

After making changes in all the files in the terminal execute the *wmake* command to compile the code, In the *controlDict* file add the following code to access the custom drag model in the simulation.

libs ("libIshiiZuberModvModel.so");