

## BUMP - BUbble column Multiphase Project

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## Contents

|          |   |           |
|----------|---|-----------|
| <b>1</b> | <b>Introduction</b>   | <b>2</b>  |
| <b>2</b> | <b>Experimental Benchmark</b>   | <b>2</b>  |
| <b>3</b> | <b>Numerical Setup</b>  | <b>3</b>  |
| 3.1      | Domain and Mesh . . . . .   | 3         |
| 3.2      | Boundary Conditions . . . . .   | 4         |
| 3.3      | Working fluids and operating conditions . . . . .                         | 4         |
| 3.4      | Turbulence modeling . . . . .   | 5         |
| 3.4.1    | $k - \omega$ SST Sato . . . . .   | 5         |
| 3.4.2    | Lahey $k - \epsilon$ . . . . .  | 5         |
| 3.4.3    | Mixture $k - \epsilon$ . . . . .  | 5         |
| 3.5      | Solver settings . . . . .   | 5         |
| 3.6      | Phase interaction modeling . . . . .                                      | 6         |
| 3.6.1    | Virtual mass force . . . . .  | 6         |
| 3.6.2    | Drag force . . . . .  | 6         |
| 3.6.3    | Lift force . . . . .  | 7         |
| 3.6.4    | Turbulent dispersion . . . . .  | 7         |
| 3.6.5    | Wall lubrication . . . . .  | 8         |
| <b>4</b> | <b>Results and Discussion</b>   | <b>8</b>  |
| 4.1      | CFD methodology . . . . .   | 8         |
| 4.2      | Mesh sensitivity . . . . .  | 8         |
| 4.3      | Time sensitivity . . . . .  | 10        |
| 4.4      | Turbulence models . . . . .   | 11        |
| 4.5      | Lift models . . . . .   | 12        |
| 4.6      | Turbulent dispersion models . . . . .                                     | 12        |
| 4.7      | Wall lubrication models . . . . .   | 13        |
| 4.8      | Inflow velocity . . . . .   | 14        |
| <b>5</b> | <b>Local results</b>  | <b>15</b> |
| <b>6</b> | <b>Conclusion</b>   | <b>15</b> |
| <b>A</b> | <b>Appendix A: fvModels source code for degassing boundary conditions</b> | <b>17</b> |

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## 1. Introduction

Bubble columns are multiphase reactors where the dispersed phase (gas) is introduced into a stationary or flowing liquid (continuous phase) and provide a good experimental setup to study the turbulent phenomena in dense bubbly flows. The functioning is apparently simple, as the ascending gas-phase creates a buoyancy-driven flow inducing the recirculation of the liquid phase. The local and the global fluid dynamic properties are related to the prevailing flow regime which may be homogeneous (bubbly flow condition at low superficial gas velocity, typically  $U_G < 0.03 \text{ m/s}$ ) or heterogeneous (churn-turbulent flow condition,  $U_G > 0.1 \text{ m/s}$ ,  $\alpha_G \geq 0.3$ ). The homogeneous flow regime can be classified into the *mono-dispersed homogeneous* flow regime, characterized by a mono-dispersed bubble size distribution (BSD), and the *pseudo-homogeneous* flow regime, characterized by a poly-dispersed BSD. The distinction between mono-dispersed and poly-dispersed BSDs is based upon the change in the sign of the lift force coefficient.

Numerous industrial designs have been based on empirical correlations, but such approaches remain somewhat limited when increasing the reactor performance is sought. To improve the description of the physical phenomenon occurring in bubble columns a promising numerical method is the Computational Fluid Dynamics (CFD). CFD helps to understand the complex two-phase fluid dynamics in the bubble column through details of mean flows (fields of three components of mean velocities and mean gas hold-up), interphase rates of mass, energy and momentum transfer and turbulence parameters (such as turbulent kinetic energy, energy dissipation rate, Reynolds stresses, etc.).

In the present work, bubble column is numerically simulated by using the open source CFD tool OpenFOAM [1]. More in detail, the objective of this work is the validation of the already existing *multiphaseEulerFoam* solver working for the case of *mono-dispersed homogeneous* bubble column. For the case study we have considered a multiphase mixture of air and water without taking into account the heat transfer phenomena.

The structure of the report is as follows. In Section 2, the experimental benchmark taken as reference is illustrated. In Section 3, all details related to the numerical setup are delineated. In Section 4, the results are discussed. Conclusions and further development are outlined in Section 5.

## 2. Experimental Benchmark

The experimental benchmark taken as reference for the validation comes from the literature, in particular from the study of Krepper et al. [2]. The experimental setup consists of three rectangular channels  $20\text{cm}^2$  in cross-section ( $0.1 \times 0.02 \text{ m}$ ) bolted together at the flanges resulting in a bubble column of 1.5-meter height (Figure 1). The test facility is initially filled with water up to 1-meter in height. In the bottom of the test section is present a rectangular porous stone adopted as gas sparger  $0.02\text{m}$  wide,  $0.01\text{m}$  depth and  $0.01\text{m}$  height. This sparger produced a *mono-dispersed homogeneous* bubble size distribution with a bubble diameter of  $3 \text{ mm}$ . The superficial gas flow rate,  $U_G$ , is varied between three different value,  $0.006 \text{ m/s}$ ,  $0.008 \text{ m/s}$  and  $0.010 \text{ m/s}$ , in the *mono-dispersed homogenous* flow regime. The superficial velocity is calculated from the measured volume flow rates using:

$$U_G = \frac{Q_G}{A_{CS}} \quad (1)$$

where  $Q_G$  is the measured volume flow rate of the gas and  $A_{CS}$  is the cross-sectional area of the test section. The column operates in the dispersed bubble bubbly regime, characterized by the absence of bubble coalescence or breakup, for the superficial gas velocities adopted in this work. For each superficial gas velocity the volume average void fraction,  $\alpha_V$ , also known as *gas holdup*, can be calculated using:

$$\alpha_V = \frac{h_{final} - h_{initial}}{h_{final}} \quad (2)$$

where  $h_{final}$  is the heighth of the liquid column after the column has been aerated and  $h_{initial}$  is the stationary height of the liquid column before aeration. The experimental data consist of wire-mesh local void fraction measurements performed at two different axial heights  $y = 0.08 \text{ m}$  and  $y = 0.63 \text{ m}$  above the gas sparger. The wire mesh sensor is placed in the cross-section by bolting it to two flanged rectangular channels. The wire-mesh sensor data was recorded at a frequency of 2500 Hz for a time period of 60 s.

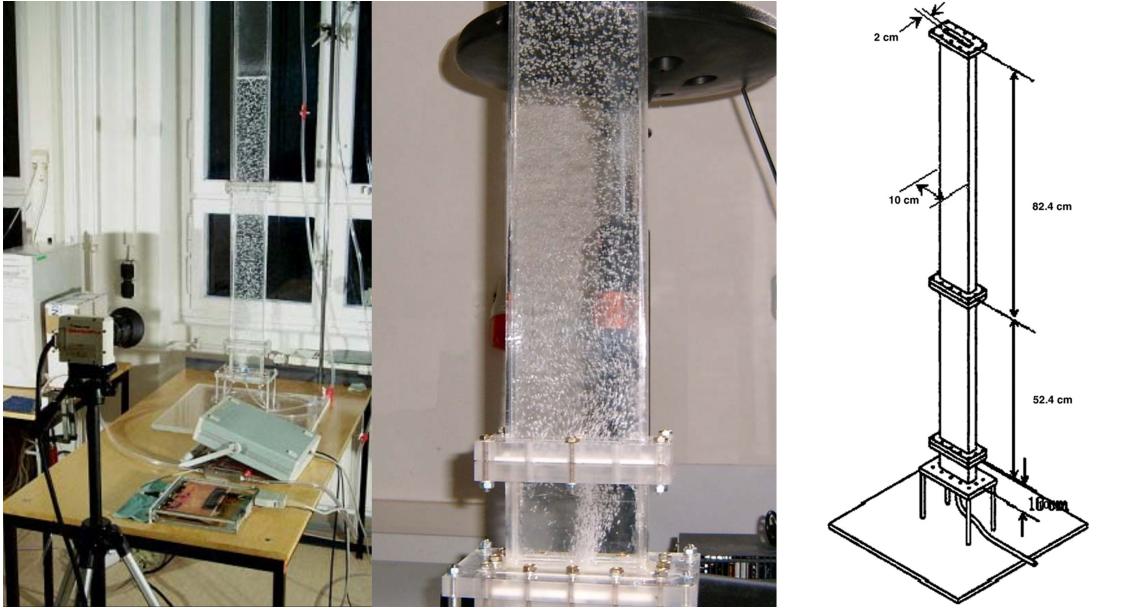


Figure 1: Pictures of the experimental setup and dimensions of the test facility.

### 3. Numerical Setup

In this section all the details related to the numerical setup will be presented and discussed.

#### 3.1. Domain and Mesh

The numerical domain has been modeled and meshed with the utility `blockMesh` according to the size of the experimental facility reported in section 2. The resulting mesh is structured and made of only regular hexahedral elements. Four different refinement levels were analyzed for the purpose of a grid sensitivity analysis. Figure 2 displays a section of the generated meshes and their details are instead summarized in table 1. According to [2], the mesh size should be 1.5 times the size of the bubbles. Therefore, given the size distribution found in the experiments (see section 2), the coarsest mesh should be the most adequate since it has a cell size of 5mm in each direction. The grid refinement study has the purpose of verify if such a coarse mesh has negative influence on the fluid-dynamic phenomena inside the bubble column.

Speaking about the inlet section, the porous stone used as gas sparger in the experiments has been modeled as a zero-thickness surface having the size of the sparger itself, namely a  $0.02 \times 0.01 \text{ m}^2$  cross-section.

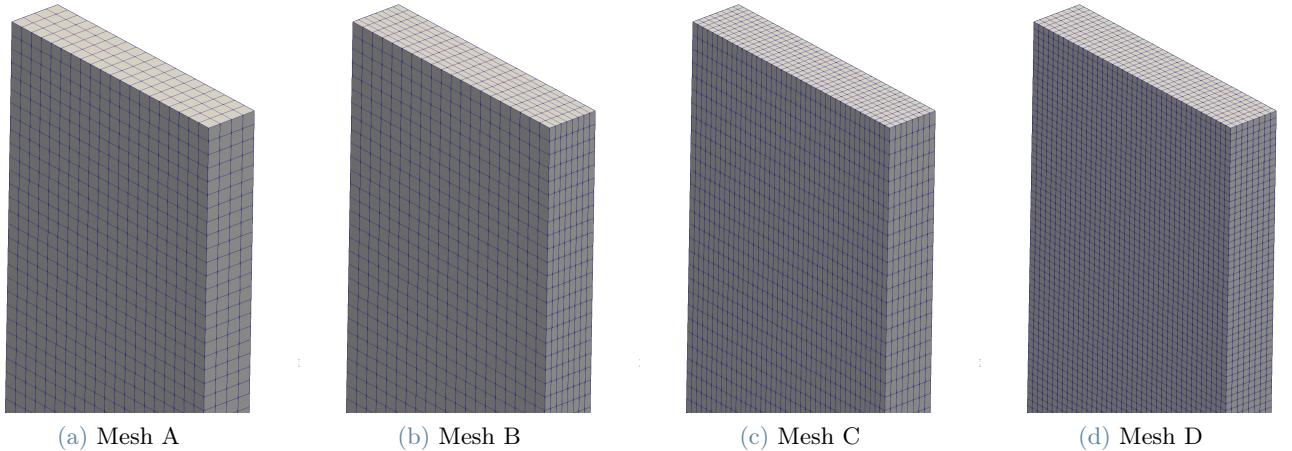


Figure 2: Different mesh densities considered in the analysis

|               | $N_x$ | $N_y$ | $N_z$ | Total no. of elements |
|---------------|-------|-------|-------|-----------------------|
| <b>Mesh A</b> | 20    | 200   | 4     | 16000                 |
| <b>Mesh B</b> | 20    | 200   | 8     | 32000                 |
| <b>Mesh C</b> | 40    | 200   | 8     | 64000                 |
| <b>Mesh D</b> | 40    | 400   | 8     | 128000                |

Table 1: Mesh size details

### 3.2. Boundary Conditions

The list of boundary conditions applied to the domain is summarized in table 2. At the inlet, three different gas superficial velocities were applied according to the three cases studied, respectively 6, 8 and 10 mm/s. These superficial velocities are an experimental input and were calculated as the volumetric flow rate of gas injected in the column divided by its volume. In OpenFOAM, a `flowRateInletVelocity` boundary condition was employed. This requires a mass flow rate input and a reference density in order to calculate the inlet velocity. The chosen density was 1.185 kg/m<sup>3</sup> which corresponds to air density at ambient conditions of 25°C and 1 atm.

Moreover, a custom `fvModels` boundary condition was developed to implement a degassing boundary condition. The complete listing of the source code is provided in Appendix A. Typically, a this type boundary condition is used to model a free surface through which dispersed gas bubbles are allowed to escape, but the continuous phase is not. A typical application is a bubble column in which the user want to reduce computational cost by not including the freeboard region in the simulation [3]. This boundary conditions offers also an improvement in terms of numerical stability since the water-air interface is not modeled. When the degassing boundary condition is specified for an outlet, the continuous liquid phase sees the boundary as a free-slip wall and does not leave the domain. The dispersed gas phase sees the boundary as an outlet. The code provided calculates an implicit mass source term to remove gas phase from the cells adjacent to the outlet boundary and also computes a degassing force to account for the effect of gas removal on the continuous phase. By adding the degassing boundary condition, the gas holdup of the entire bubble column can be simply calculated as the void fraction of air in the entire domain.

| Variable      | Inlet                 | Outlet                      | Walls               |
|---------------|-----------------------|-----------------------------|---------------------|
| alpha.air     | fixedValue            | zeroGradient                | zeroGradient        |
| alpha.water   | fixedValue            | zeroGradient                | zeroGradient        |
| k.water       | fixedValue            | inletOutlet                 | kqRWallFunction     |
| epsilon.water | fixedValue            | inletOutlet                 | epsilonWallFunction |
| omega.water   | fixedValue            | inletOutlet                 | omegaWallFunction   |
| km            | fixedValue            | inletOutlet                 | kqRWallFunction     |
| epsilonnm     | fixedValue            | inletOutlet                 | epsilonWallFunction |
| nut.water     | calculated            | calculated                  | nutkWallFunction    |
| p             | calculated            | calculated                  | calculated          |
| U.air         | flowRateInletVelocity | pressureInletOutletVelocity | fixedValue          |
| U.water       | fixedValue            | slip                        | fixedValue          |

Table 2: List of boundary conditions applied to the three different boundaries

### 3.3. Working fluids and operating conditions

In order to model the bubble column, a two-phase mixture made of air and water was considered. As reported in section 2, the experimental setup provided a monodispersed bubble size distribution with a mean equivalent diameter of 3mm. The dispersed phase is therefore modeled by using a single gas phase considering only small

bubbles. Despite the air phase having a slightly varying density from the bottom to the top of the column, both fluids are considered incompressible. Table 3 summarizes material properties of both phases. The column was simulated at ambient pressure of  $10^5$  Pa with gravitational acceleration acting along Z coordinate. The system was considered isothermal and no thermophysical property was dependent on temperature. No heat nor mass transfer was considered between phases.

| Phase         | Property          | Type     | Value                      |
|---------------|-------------------|----------|----------------------------|
| Air           | Density           | Constant | 1.185 [kg/m <sup>3</sup> ] |
| Water         | Density           | Constant | 998.0 [kg/m <sup>3</sup> ] |
| Air           | Bubble diameter   | Constant | 3 [mm]                     |
| Air and water | Surface Tension   | Constant | 0.072 [N/m]                |
| Air           | Eötvös number     | Constant | 1                          |
| Air           | Dynamic viscosity | Constant | 1.84e-05 [Pa/s]            |
| Water         | Dynamic viscosity | Constant | 3.65e-04 [Pa/s]            |

Table 3: List of boundary conditions applied to the three different boundaries

### 3.4. Turbulence modeling

#### 3.4.1 $k - \omega$ SST Sato

The  $k - \omega$  SST Sato model [4] was originally developed to tackle the problem of heat transfer for boundary layer flows. It combines eddy-viscosity models for the momentum equations and eddy-diffusivity model for heat transfer. The idea behind SST model is to combine the best elements of the  $k - \epsilon$  model and the  $k - \omega$  model with the help of a blending function. Indeed, the  $k - \epsilon$  model presents deficiencies near the wall, where fine meshes and specific near-wall treatments are required. Whereas, the  $k - \omega$  model is strongly dependent of the solution to free stream values of  $\omega$  outside the boundary layer. In addition Sato [5] model for bubble induced turbulence viscosity was added to this turbulence model especially for tackling multiphase problems.

#### 3.4.2 Lahey $k - \epsilon$

This  $k - \epsilon$  model has been developed by Lahey [6] specifically for three-dimensional, four-field, turbulent, two-fluid multiphase flows. It is an extension to two-phase flows of the standard single-phase  $k - \epsilon$  turbulence model.

#### 3.4.3 Mixture $k - \epsilon$

The Mixture  $k - \epsilon$  model [7] has been developed to overcome the limitations of the standard  $k - \epsilon$  turbulence model in the application to dilute systems.

As the phase fraction increases, the dominance of the continuous phase on turbulence gradually diminishes as that phase becomes confined to thin interstices between dispersed phase elements. In the limit of unity dispersed phase fraction, this phase becomes continuous and its turbulence becomes the dominant/sole factor.

The Mixture  $k - \epsilon$  model appropriately incorporate high phase regimes and reverts to the single-phase form in the extreme limits of zero and unity phase fractions.

### 3.5. Solver settings

The *multiphaseEulerFoam* solver enables simultaneous modelling of complex multiphase flows with different flow regimes. Usually the VOF interface capturing method is used to model the large fluid-fluid interfaces, whereas in our case the Euler multi-fluid approach is used for modelling the dispersed flow. In the Euler multi-fluid approach each phase is represented by separate set of flow equations. The multi-fluid model governing equations for compressible, isothermal flow are given by a set of mass and momentum equations for each phase  $i$ :

$$\frac{\partial \alpha_i}{\partial t} + u_i \cdot \nabla(\alpha_i) = 0 \quad (3)$$

$$\frac{\partial \rho_i \alpha_i u_i}{\partial t} + \rho_i \alpha_i u_i \cdot \nabla u_i = -\alpha_i \nabla p + \nabla \cdot (\mu_i \alpha_i \nabla u_i) + F_g + F_{D,i} + F_i \quad (4)$$

where  $\alpha_i$  is the phase fraction,  $\rho_i$  the density,  $u_i$  the velocity each for the respective phase  $i$  and  $F_g$  is the gravitational force. The two interfacial forces are the drag force  $F_{D,i}$  and  $F_i$  represents all the other multiphase forces.

The first step is to define the properties of each compressible fluid phases with common pressure. Subsequently, the phase transport equations are solved for each individual phases and are calculated the interface properties of different phase pairs. The flow equations are solved through the use of the PIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm. Different sub-models are used for defining interfacial properties between each individual phase pairs for example the `dragModel`. In Table 4 and 5 are summarized the choices made.

| Mathematical term    | Numerical scheme           |
|----------------------|----------------------------|
| ddtSchemes           | backward                   |
| gradSchemes          | cellLimited Gauss linear 1 |
| divSchemes           | Gauss vanLeer              |
| laplacianSchemes     | Gauss linear limited 1     |
| interpolationSchemes | linear                     |
| snGradSchemes        | limited 1                  |

Table 4: List of numerical schemes adopted for the different mathematical terms in the **fvSchemes** file.

| Variable                  | Solver               | Smoothen              | Tolerance              |
|---------------------------|----------------------|-----------------------|------------------------|
| U, k, epsilon, omega<br>p | smoothSolver<br>GAMG | symGaussSeidel<br>DIC | $10^{-7}$<br>$10^{-8}$ |

| Correctors           |        | Relaxation factors |            |
|----------------------|--------|--------------------|------------|
| alpha<br>PIMPLE loop | 1<br>2 | p<br>All equations | 0.3<br>0.5 |

Table 5: List of entries adopted in the **fvSolution** file for both the air and water.

### 3.6. Phase interaction modeling

Interfacial forces between bubbles and liquid are of fundamental importance when modeling a multiphase system. They are responsible of momentum transfer between phases in the Eulerian framework. Therefore, their careful modeling is directly linked to the accuracy of the results. Several forces are acting on a bubble in a multiphase system. They are: virtual mass force, drag, lift, turbulent dispersion and wall lubrication forces. In the next paragraphs a brief description of each force is given.

#### 3.6.1 Virtual mass force

The virtual mass force describes resistance to relative acceleration. It occurs when a secondary phase accelerates relative to the primary phase. The inertia of the primary-phase mass encountered by the accelerating particles (or droplets or bubbles) exerts a "virtual mass force" on the particles. Its formulation is fairly simple and it is given in equation 5

$$\vec{F}_{VM} = C_{VM} \alpha_p \rho_q \left( \frac{d_q \vec{v}_q}{dt} - \frac{d_p \vec{v}_p}{dt} \right) \quad (5)$$

$$C_{VM} = 0.5$$

#### 3.6.2 Drag force

This force models is used to describe the resistance acting on the bubble due to relative motion in the fluid (primary phase). In this work the simulations were performed using the drag model developed by Ishii and Zuber in [8]. This a very complete drag model that accounts for bubble deformation. In fact, depending on

Eötvös number, a rising bubble can have a spherical shape, an elliptic one or deforming to a spherical cap. Ishii and Zuber's model models the drag coefficient as:

$$\begin{aligned}
C_D &= \max(C_{D, \text{sphere}}, \min(C_{D, \text{ellipse}}; C_{D, \text{cap}})) \\
C_{D, \text{sphere}} &= \frac{24}{Re_P} (1 + 0.1 Re_P^{0.75}) \\
C_{D, \text{ellipse}} &= \frac{2}{3} \sqrt{Eo} \\
C_{D, \text{cap}} &= \frac{8}{3}
\end{aligned} \tag{6}$$

### 3.6.3 Lift force

The lift force describe migration of bubble in shear flow act on a particle mainly due to velocity gradients in the primary phase flow field. The expression of the lift force on a secondary phase  $p$  in a primary phase  $q$  is given by:

$$\vec{F}_{lift} = -C_l \rho_q \alpha_p (\vec{v}_q - \vec{V}_p) \times (\nabla \times \vec{V}_q) \tag{7}$$

In this work two main lift model were tested: Moraga's [9] and Tomiyama's [10].

The first one was developed for solid spherical particles but can be employed also for spherical bubbles. In this model two contribution to the lift force are accounted for: the classical aerodynamic one and the vorticity-induced lift. Its formulation is given in equation 8.

$$C_l = - \left( 0.12 - 0.2 e^{-(\varphi/3.6) \times 10^{-5}} \right) e^{(\varphi/3) \times 10^{-7}} \quad 6000 < \varphi < 5 \times 10^7$$

where  $\varphi = Re_p Re_\omega$  and

$$\begin{aligned}
Re_p &= \frac{\rho_q |\vec{V}_q - \vec{V}_p| d_p}{\mu_q} \\
Re_\omega &= \frac{\rho_q |\nabla \times \vec{V}_q| d_p^2}{\mu_q}
\end{aligned} \tag{8}$$

Tomiyama's models, instead, can be applied also to deformed bubbles. Its main feature is prediction of the cross-over point in bubble size at which particle distortion causes a reversal in the sign of the lift force. Bubbles with a diameter larger than about 5.8mm have negative lift coefficient and move towards the center of the column while small ones move towards the walls. Equation 9 shows the fundamental equations of this model.

$$\begin{aligned}
C_L &= \begin{cases} \min[0.288 \tanh(0.121 Re_P), f(Eo_\perp)] & \text{for } Eo_\perp < 4 \\ f(Eo_\perp) & \text{for } 4 < Eo_\perp < 10 \\ -0.27 & \text{for } 10 < Eo_\perp \end{cases} \\
f(Eo_\perp) &= 0.00105 Eo_\perp^3 - 0.0159 Eo_\perp^2 - 0.0204 Eo_\perp + 0.474
\end{aligned} \tag{9}$$

$$Eo_\perp = \frac{g(\rho_C - \rho_D) d_\perp^2}{\sigma}$$

### 3.6.4 Turbulent dispersion

This force accounts for the interphase turbulent momentum transfer. The turbulent dispersion force acts as a turbulent diffusion in dispersed flows. The model considered in this report and the ones by Lopez de Bertodano [11] and Burns [12]. Thir formulation is reported in equations 10 and 11 respectively.

$$\vec{F}_{td,q} = -\vec{F}_{td,p} = C_{TD} \rho_q k_q \nabla \alpha_p \tag{10}$$

$$\vec{F}_{td,q} = -\vec{F}_{td,p} = C_{TD} K_{pq} \frac{D_q}{\sigma_{pq}} \left( \frac{\nabla \alpha_p}{\alpha_p} - \frac{\nabla \alpha_q}{\alpha_q} \right) \tag{11}$$

### 3.6.5 Wall lubrication

It describes migration of bubble away from the walls due to the presence of the walls themselves. This results in the dispersed phase concentrating in a region near but not adjacent to the walls. The general expression of the wall lubrication force acting on a secondari phase  $p$  in a primary phase  $q$  is given by:

$$\vec{F}_{wl} = C_{wl}\rho_q\alpha_p \left|(\vec{v}_q - \vec{v}_p)_{||}\right|^2 \vec{n}_w \quad (12)$$

where  $C_{wl}$  is the wall lubrication coefficient and  $\vec{n}_w$  the unit normal to the wall.

In this work tow different models between the ones already available in openFOAM were considered: Antal's [13] and Frank's one [14].

The first one computes the wall lubricaton coefficient as

$$C_{wl} = \max \left( 0, \frac{C_{w1}}{d_b} + \frac{C_{w2}}{y_w} \right) \quad (13)$$

where  $C_{w1}$  and  $C_{w2}$  are non-dimensional coefficients and  $y_w$  is the distance to the nearest wall.

Frank's model, instead, computes  $C_{wl}$  as

$$C_{wl} = C_w \max \left( 0, \frac{1}{C_{wd}} \cdot \frac{1 - \frac{y_w}{C_{wd} d_b}}{y_w \left( \frac{y_w}{C_{wd} d_b} \right)^{m-1}} \right) \quad (14)$$

where  $C_{wd}$ ,  $C_{wc}$  and  $m$  are calibration coefficients.

## 4. Results and Discussion

In this section the results of the present work are presented and commented. Each subsection represents the sensitivity analysis on some parameters which may or may not influence the numerical results. The analysis performed aim at evaluating the sensitivity of the CFD results on the mesh, timestep and each multiphase force in this order.

### 4.1. CFD methodology

All the simulations are three-dimensional and time-dependent. The solution was initialized with constant pressure distribution at  $P_{atm}$  and the bubble column was filled with water. The simulated time was 90 seconds for each case. Results were averaged from 30 s to the end of the simulations in order to obtain the averaged field in terms of velocity, pressure and void fraction distribution for both phases. In particular, the air void fraction was sampled on two horizontal surfaces at 8 cm and 63 cm height from the inlet surface in order to compare the numerical results to the experimental ones. Benchmark for the accuracy of the simulations are therefore the time-averaged distribution of local gas hold up profile on the two horizontal surfaces as well as the global gas holdup value of the entire bubble column (referred to as "numerical holdup" in the following tables). Table 6 summarizes all the runs performed.

### 4.2. Mesh sensitivity

The sensitivity analysis on mesh refinement has the objective of evaluating how the cell dimension influence the accuracy of the results. In this work we considered four different mesh sizes doubling the number of elements in Z, X and Y direction respectively. This sensitivity analysis was conducted considering a base case with just the influence of drag and lift force as reported in table 6.

|        | $J_{in}$ [mm/s] | Mesh | Time step | Turbulence model | Drag model | Lift model | Turbulent dispersion model | Wall lubrication model |
|--------|-----------------|------|-----------|------------------|------------|------------|----------------------------|------------------------|
| run001 | 10              | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | None                       | None                   |
| run002 | 10              | B    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | None                       | None                   |
| run003 | 10              | C    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | None                       | None                   |
| run004 | 10              | D    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | None                       | None                   |
| run005 | 10              | A    | 0.010     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | None                       | None                   |
| run006 | 10              | A    | 0.0025    | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | None                       | None                   |
| run007 | 10              | A    | 0.005     | LaheyKEpsilon    | IshiiZuber | Tomiyama   | None                       | None                   |
| run008 | 10              | A    | 0.005     | mixtureKEpsilon  | IshiiZuber | Tomiyama   | None                       | None                   |
| run009 | 10              | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | None       | None                       | None                   |
| run010 | 10              | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Moraga     | None                       | None                   |
| run011 | 10              | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | Burns                      | None                   |
| run012 | 10              | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | LopezDeBertodano           | None                   |
| run013 | 10              | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | Burns                      | Antal                  |
| run014 | 10              | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | Burns                      | Frank                  |
| run015 | 8               | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | Burns                      | Antal                  |
| run016 | 6               | A    | 0.005     | kOmegaSSSTSato   | IshiiZuber | Tomiyama   | Burns                      | Antal                  |

Table 6: Runs performed

|               |               | $N_x$ | $N_y$ | $N_z$ | Experimental holdup [-] | Numerical holdup [-] | $\Delta\varepsilon [\%]$ | Execution Time [h] |
|---------------|---------------|-------|-------|-------|-------------------------|----------------------|--------------------------|--------------------|
| <b>run001</b> | <b>Mesh A</b> | 20    | 200   | 4     | 0.03501                 | 0.04049              | 15.65                    | 3.26               |
| <b>run002</b> | <b>Mesh B</b> | 20    | 200   | 8     | 0.03501                 | 0.04116              | 17.57                    | 6.09               |
| <b>run003</b> | <b>Mesh C</b> | 40    | 200   | 8     | 0.03501                 | 0.04064              | 16.08                    | 11.72              |
| <b>run004</b> | <b>Mesh D</b> | 40    | 400   | 8     | 0.03501                 | 0.04078              | 16.48                    | 25.44              |

Table 7: Results of sensitivity analysis on mesh refinement

Figure 3 displays the trend of local gas holdup on the two reference surfaces. From this plots we can observe virtually no difference between all the cases. It is worth noting that mesh size has an impact on the computational time of the simulation. It was observed that the computational time scaled almost linearly with mesh size so, given the results, the optimal choice was to choose the coarsest mesh for all the other runs.

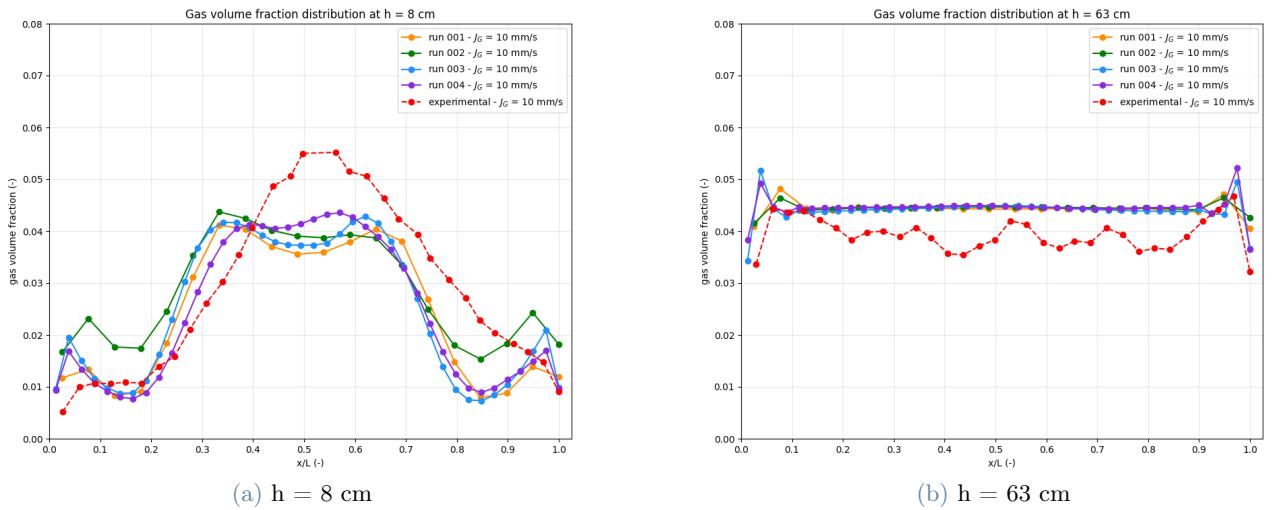


Figure 3: Gas volume fraction horizontal distribution at different heights for different meshes

### 4.3. Time sensitivity

The sensitivity analysis on timestep size has the objective of evaluating how the results can be influenced by a finer or coarser temporal discretization. To do so additional calculation halving and doubling the time step were performed. The global gas holdup shows no influence due to timestep size. It was observed, though, that the coarsest timestep gave stability problems and Courant number grater than 5 for some of the test cases so it was decided to stick with a timestep of 0.005 seconds also considering the computational time required for a simulation.

|               | $\Delta t$ | Experimental holdup [-] | Numerical holdup [-] | $\Delta\varepsilon [\%]$ |
|---------------|------------|-------------------------|----------------------|--------------------------|
| <b>run006</b> | 0.0025     | 0.03501                 | 0.04015              | 14.71                    |
| <b>run001</b> | 0.005      | 0.03501                 | 0.04049              | 15.65                    |
| <b>run005</b> | 0.010      | 0.03501                 | 0.03983              | 13.77                    |

Table 8: Results of timestep size sensitivity analysis

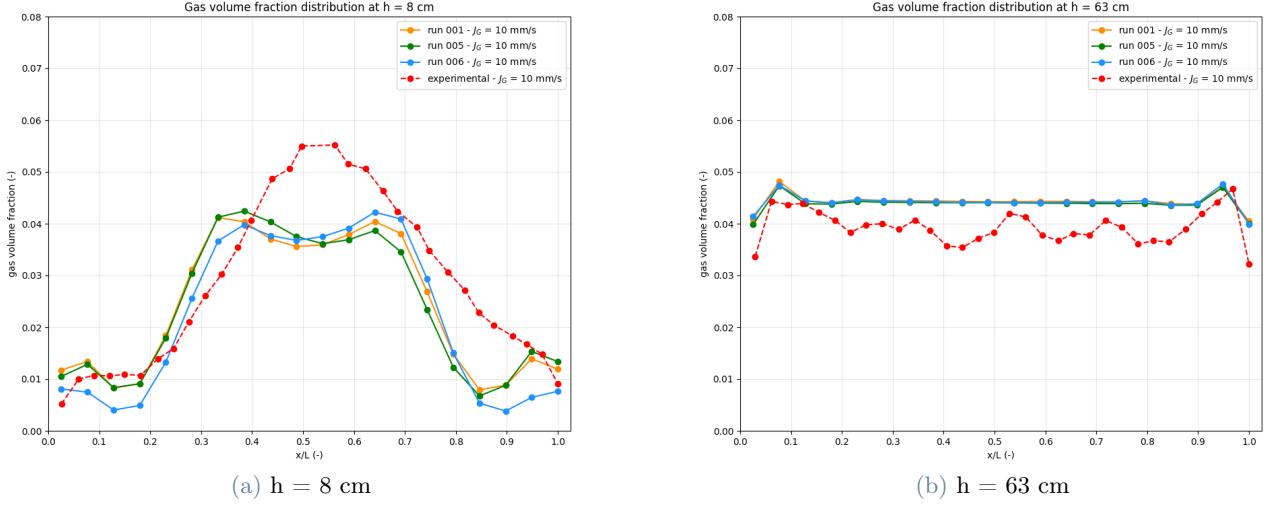


Figure 4: Gas volume fraction horizontal distribution at different heights for different time steps

#### 4.4. Turbulence models

As reported in section 3.4, different turbulence models are available for multiphase simulation. Therefore, it is important to test their influence on the results. As reported by Hänsch et al. in [15], the best strategy for solving a bubbly flow is to consider SST turbulence model and to solve for turbulence just in the continuous phase. In openFOAM, several models for multiphase turbulence prediction are available. As reported in table 9, Lahey k- $\epsilon$  models seems to be the most accurate one. Anyway, by looking at figure 5, this model overestimates the gas holdup at the center of the column in the developed region while the other two are more adherent to experimental data. The mixture k- $\epsilon$  instead, has two main disadvantages. The first one is that it is not possible to account for turbulence just in the continuous phase and it does not provide a model for bubble turbulence interaction (BIT). The k- $\omega$  SST provides the Sato model for this scope and it must therefore be preferred.

| Turbulence model | Experimental holdup [-] | Numerical holdup [-] | $\Delta\epsilon$ [%] |
|------------------|-------------------------|----------------------|----------------------|
| <b>run001</b>    | kOmegaSSTSato           | 0.03501              | 0.04049              |
| <b>run007</b>    | LaheyKEpsilon           | 0.03501              | 0.03883              |
| <b>run008</b>    | mixtureKEpsilon         | 0.03501              | 0.03986              |

Table 9: Results of turbulence models sensitivity analysis

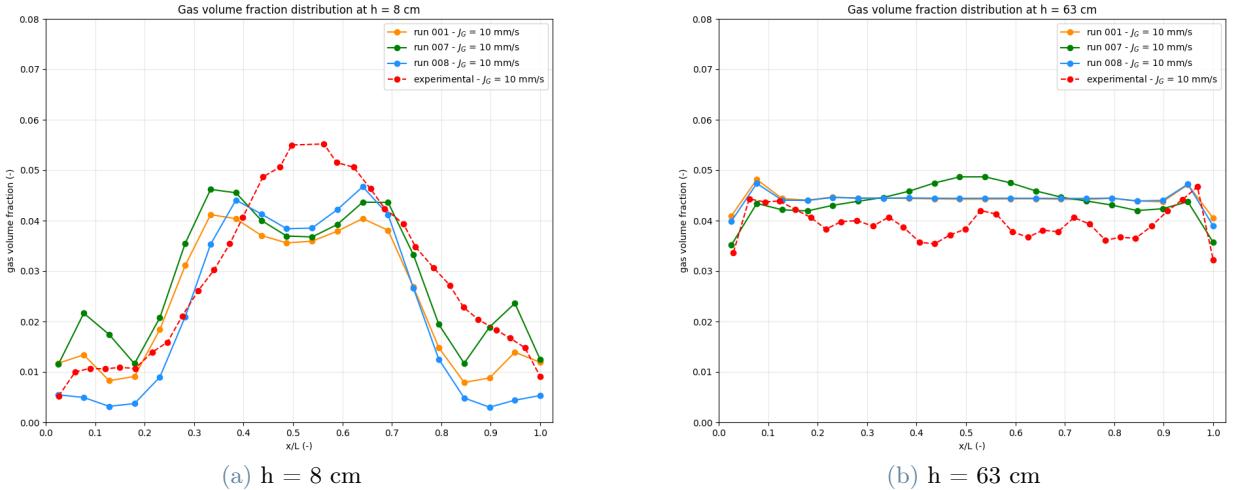


Figure 5: Gas volume fraction horizontal distribution at different heights for different turbulence models

## 4.5. Lift models

The lift force in a bubble column is responsible of lateral forces and oscillation of the bubble swarm. It is therefore an important force that should not be neglected. In this sensitivity analysis two models are tested and also the effect of lift absence is shown. Tomiyama model is the least accurate in terms of global holdup but it is the one which represents the local air void fraction profile. By looking at figure 6, the effect of neglecting the lift force is clearly visible. The bubbles are concentrated in the center of the column and the holdup profile assumes an almost parabolic shape in the developed region. This is due to the lack of lateral forces that make the bubble swarm oscillate. The Moraga model, is similar to Tomiyama's one in terms of holdup profile but it slightly overpredicts the air void fraction in the center of the column. Moreover, as explained in section 4.5, it is lacking the Tomiyama's model feature of variable lift force direction depending on bubble size. In conclusion the Tomiyama model is the most suitable for this kind of simulations.

| Lift model | Experimental holdup [-] | Numerical holdup [-] | $\Delta\varepsilon [\%]$ |
|------------|-------------------------|----------------------|--------------------------|
| run009     | None                    | 0.03501              | 0.03111                  |
| run001     | Tomiyama                | 0.03501              | 0.04049                  |
| run010     | Moraga                  | 0.03501              | 0.03950                  |

Table 10: Results of lift models sensitivity analysis

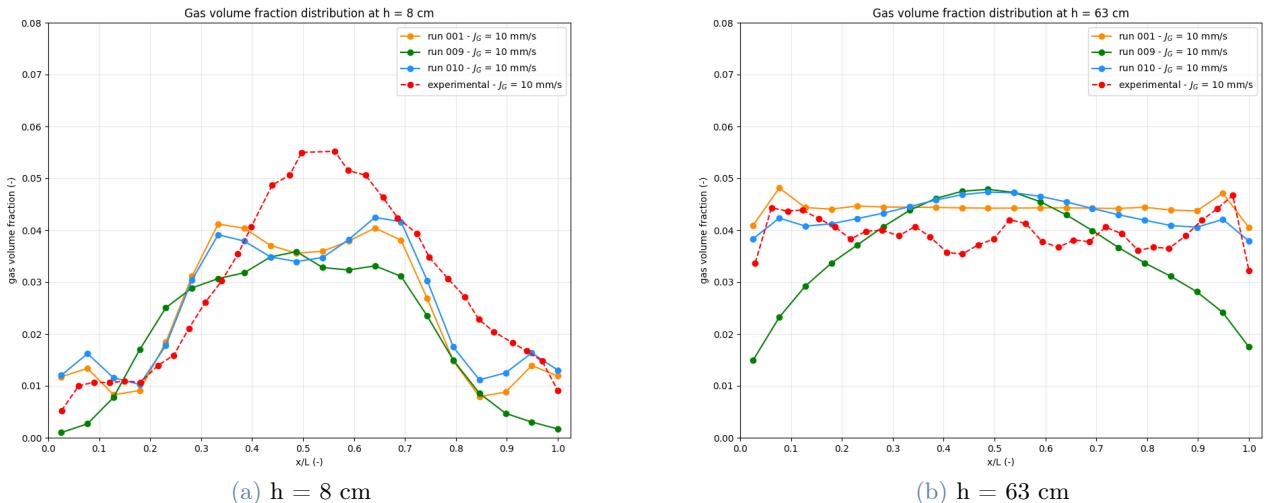


Figure 6: Gas volume fraction horizontal distribution at different heights for different lift models

## 4.6. Turbulent dispersion models

This force accounts for the interphase turbulent momentum transfer. By looking at table 11, one could say that considering this force in the analysis has a negative impact on the accuracy. This is not true when considering the local holdup profile displayed in figure 7. In the injection zone ( $h=8\text{cm}$ ) the profile is very close to the experimental one. This is the first case that exhibits a parabolic shape profile instead of a concave one. Both models are close to the experimental lines and resemble its shape. Lopez de Bertodano's model though, overestimates the gas holdup profile. This trend is reflected on the numerical value of the global holdup which reaches an error level of 31%. Therefore, given the results discussed, Burns model was chosen for the remaining simulations.

| Turbulent dispersion model |                  | Experimental holdup [-] | Numerical holdup [-] | $\Delta\varepsilon [\%]$ |
|----------------------------|------------------|-------------------------|----------------------|--------------------------|
| <b>run001</b>              | None             | 0.03501                 | 0.04049              | 15.65                    |
| <b>run011</b>              | Burns            | 0.03501                 | 0.04285              | 22.39                    |
| <b>run012</b>              | LopezDeBertodano | 0.03501                 | 0.0459               | 31.11                    |

Table 11: Results of sensitivity analysis on turbulent dispersion models

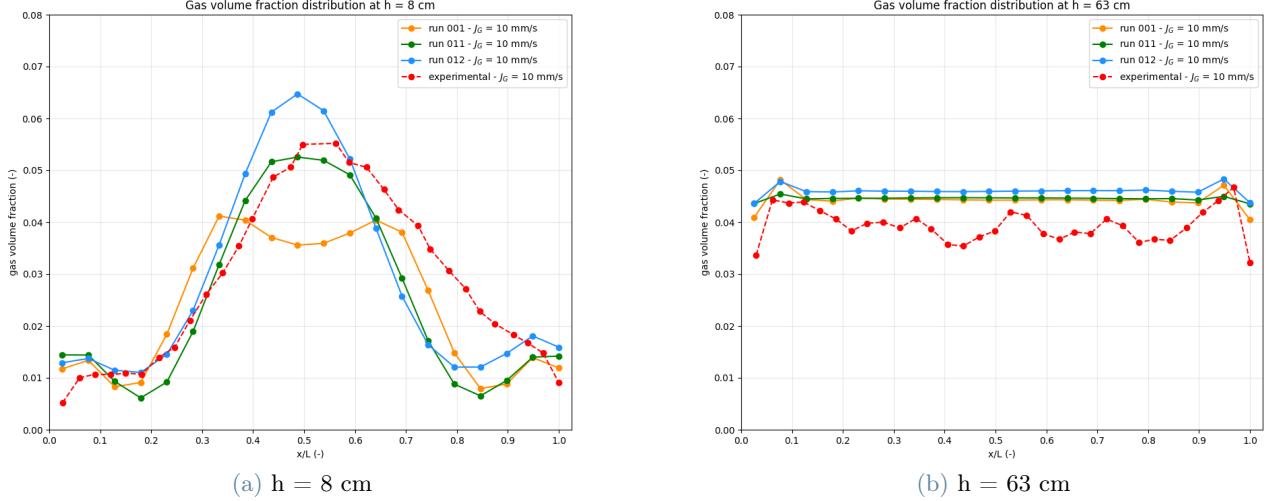


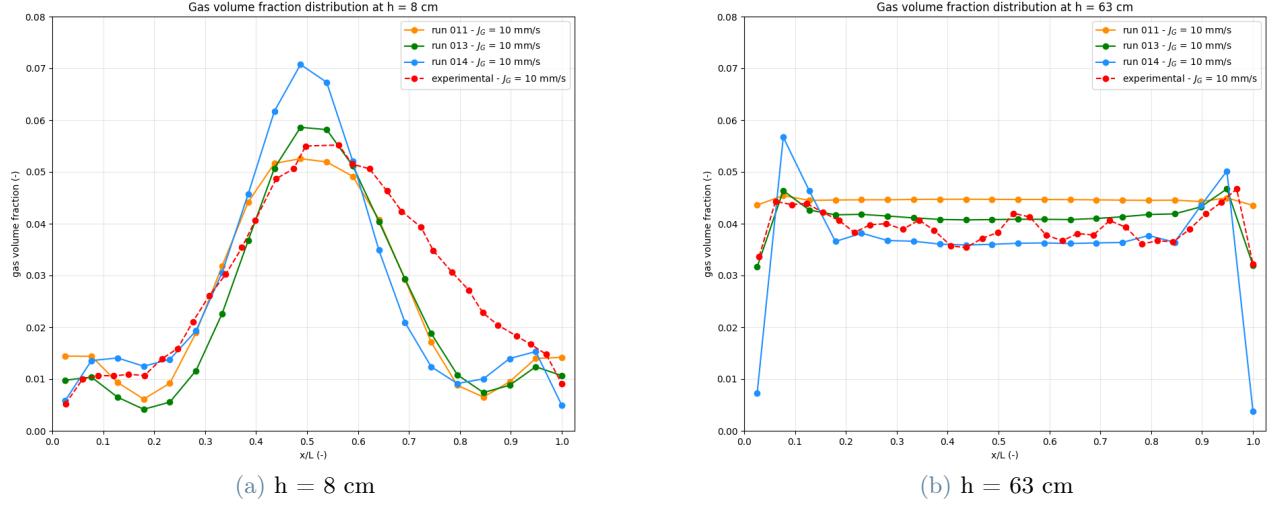
Figure 7: Gas volume fraction horizontal distribution at different heights for different turbulent dispersion models

#### 4.7. Wall lubrication models

This force describes migration of bubble away from the walls due to the presence of the walls themselves. This effect is particularly visible in figure 8. By looking at the developed region ( $h=63$  cm) far from the inlet, is it clearly visible that Frank's model predicts a too strong wall lubrication force. The first point away from the wall sees a very low air void fraction which reaches instead a peak slightly away from the wall itself. This is reflected in the very low global gas holdup predicted when using this model. Antal model instead, has a softer behavior and it matches the experimental results almost perfectly in terms of local holdup profile. In the injection zone this force does not have a great impact on the results since the bubble are concentrated in the central region of the bubble column.

| Wall lubrication model |       | Experimental holdup [-] | Numerical holdup [-] | $\Delta\varepsilon [\%]$ |
|------------------------|-------|-------------------------|----------------------|--------------------------|
| <b>run001</b>          | None  | 0.03501                 | 0.04049              | 15.65                    |
| <b>run013</b>          | Antal | 0.03501                 | 0.04014              | 14.65                    |
| <b>run014</b>          | Frank | 0.03501                 | 0.03061              | -12.57                   |

Table 12: Results of sensitivity analysis on wall lubrication models



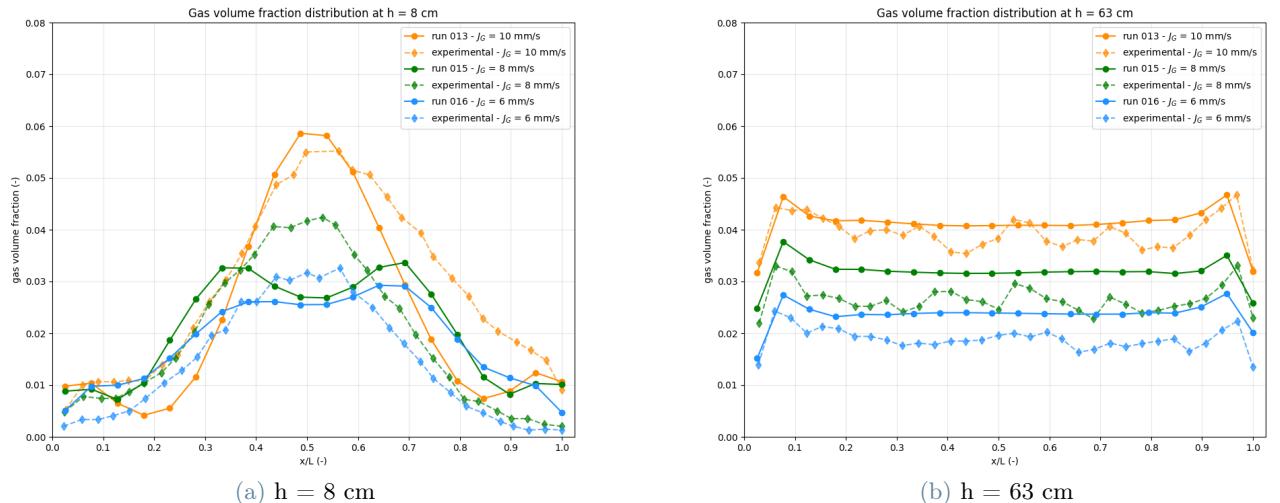
**Figure 8:** Gas volume fraction horizontal distribution at different heights for different wall lubrication models

#### 4.8. Inflow velocity

Once defined the optimal set of condition, additional experimental results at different gas superficial inlet velocity were considered. The approach remains valid also for lower gas inlet velocities. The error on global holdup is between 10% and 15% for all three cases. The local holdup profiles are in good agreement with experimental data, especially in the developed region.

|               | $J_{in} [\text{mm/s}]$ | Experimental holdup [-] | Numerical holdup [-] | $\Delta\varepsilon [\%]$ |
|---------------|------------------------|-------------------------|----------------------|--------------------------|
| <b>run013</b> | 10                     | 0.03501                 | 0.04014              | 14.65                    |
| <b>run015</b> | 8                      | 0.02808                 | 0.03098              | 10.33                    |
| <b>run016</b> | 6                      | 0.02042                 | 0.02273              | 11.31                    |

**Table 13:** Results obtained at different inflow gas superficial velocities



**Figure 9:** Gas volume fraction horizontal distribution at different heights for different inflow velocities

## 5. Local results

Post-processing...

## 6. Conclusion

The present work had the objective of validating openFOAM multiphase capabilities against experiments. A bubble column from literature was considered as experimental benchmark. Simulations showed that mesh and timestep refinement have little influence on the accuracy of the results. The SST turbulence model resulted the best one when considering the holdup profiles as well as the capabilities of the turbulence models itself. For what concerns the multiphase forces, it was showed how important it is to evaluate carefully their use in the numerical model. By adding the various forces in a step-by-step manner and evaluating their impact on the results, an optimal configuration was defined and it is summarized in table 14. In conclusion, openFOAM and the solver `multiphaseEulerFoam` proved themselves to be a valuable tool when tackling multiphase simulations.

| Model for            |                          |
|----------------------|--------------------------|
| Turbulence           | k- $\omega$ SST Sato [4] |
| Virtual mass         | Constant = 0.5           |
| Drag                 | Ishii Zuber [8]          |
| Lift                 | Tomiyama [10]            |
| Turbulent dispersion | Burns [12]               |
| Wall lubrication     | Antal [13]               |

Table 14: Summary of the optimal multiphase forces configuration

## References

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## A. Appendix A: fvModels source code for degassing boundary conditions

```

/*----- C++ -----*/
| ====== | | OpenFOAM: The Open Source CFD Toolbox |
| \ \ / F ield | Version: 3.0.0 |
| \ \ / O peration | Web: www.OpenFOAM.org |
| \ \ / A nd | |
| \ \ \ M anipulation | |
\*----- */

FoamFile
{
    version      2.0;
    format       ascii;
    class        dictionary;
    location     "constant";
    object       fvOptions;
}

// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //

degassingMassSource
{
    type          coded;
    active        yes;
    selectionMode all;
    field         thermo:rho.air;

    name          degassingMassSource;
    patches       (outlet);
    rhoName       thermo:rho.air;
    alphaName     alpha.air;

    codeInclude
    #{
        #include "fvm.H"
    };

    codeAddRhoSup
    #{

        Info << "**codeAddSup**" << endl;

        // Get the names of the patches on which to apply the degassing forces
        DynamicList<word, 1, 0> patches;
        coeffs().lookup("patches") >> patches;

        // Get the required fields
        const word rhoName = coeffs().lookup("rhoName");
        const volScalarField& rhoAir = mesh().lookupObject<volScalarField>(rhoName);
        const word alphaName = coeffs().lookup("alphaName");
        const volScalarField& alphaAir = mesh().lookupObject<volScalarField>(alphaName);

        // Get the timestep
        const scalar deltaT = mesh().time().deltaT().value();

        // Create degassing mass source coefficient and initialize to zero
        volScalarField degassingMassSourceCoeff
        (

```

```

IOobject
(
    "degassingMassSourceCoeff",
    mesh().time().timeName(),
    mesh(),
    IOobject::NO_READ,
    IOobject::AUTO_WRITE
),
mesh(),
dimensionedScalar("degassingMassSourceCoeff", dimless/dimTime, 0.0)
);

// Compute the degassing mass source coefficient for each cell adjacent to the
selected patches
forAll(patches, iPatch)
{
    // Get the boundary patch
    const fvPatch& patch = mesh().boundary()[patches[iPatch]];

    // Loop through each boundary face and compute degassing force coefficient in
    adjacent cell
    forAll(patch, iFace)
    {
        label iCell = patch.faceCells()[iFace];
        degassingMassSourceCoeff[iCell] = -alphaAir[iCell]/deltaT;
    }
}

// Add the degassing force term
eqn += fvm::Sp(degassingMassSourceCoeff, rhoAir);
#};

codeOptions
#{

-I$(LIB_SRC)/finiteVolume/lnInclude \
-I$(LIB_SRC)/meshTools/lnInclude
#};

}

degassingForce
{
    type          coded;
    active        yes;
    selectionMode all;
    field         U.air;
    name          degassingForce;
    patches       (outlet);
    rhoName      thermo:rho.air;
    alphaName    alpha.air;
    UName        U.air;

    codeInclude
    #{
        #include "fvm.H"
    };

    codeAddRhoSup
    #{
}

```

```

// Get the names of the patches on which to apply the degassing forces
DynamicList<word, 1, 0> patches;
coeffs().lookup("patches") >> patches;

// Get the required fields
const word rhoName = coeffs().lookup("rhoName");
const volScalarField& rhoAir = mesh().lookupObject<volScalarField>(rhoName);
const word alphaName = coeffs().lookup("alphaName");
const volScalarField& alphaAir = mesh().lookupObject<volScalarField>(alphaName);
const word UName = coeffs().lookup("UName");
const volVectorField& UAir = mesh().lookupObject<volVectorField>(UName);

// Get the timestep
const scalar deltaT = mesh().time().deltaT().value();

// Create degassing force coefficient and initialize to zero
volScalarField degassingForceCoeff
(
    IOobject
    (
        "degassingForceCoeff",
        mesh().time().timeName(),
        mesh(),
        IOobject::NO_READ,
        IOobject::AUTO_WRITE
    ),
    mesh(),
    dimensionedScalar("degassingForceCoeff", dimDensity/dimTime, 0.0)
);

// Compute the degassing force coefficient for each cell adjacent to the selected
patches
forAll(patches, iPatch)
{
    // Get the boundary patch
    const fvPatch& patch = mesh().boundary()[patches[iPatch]];

    // Loop through each boundary face and compute degassing force coefficient in
    adjacent cell
    forAll(patch, iFace)
    {
        label iCell = patch.faceCells()[iFace];
        degassingForceCoeff[iCell] = -rhoAir[iCell]*alphaAir[iCell]/deltaT;
    }
}

// Add the degassing force term
eqn += fvm::Sp(degassingForceCoeff, UAir);
#};

codeOptions
#{ 
-I$(LIB_SRC)/finiteVolume/lnInclude \
-I$(LIB_SRC)/meshTools/lnInclude
#};
}

// ****

```

Listing 1: fvModels source code