
Hands-on session 12 – Bubble Column


Abstract

The purpose of this tutorial is to provide guidelines and recommendations for solving the fluid dynamics in a gas-liquid bubble column using the Eulerian multiphase model.

Goal

The purpose of this hands-on session is to provide guidelines and recommendations for solving a gas-liquid bubble column problem using the Eulerian multiphase model, including advice on model and solver settings. This tutorial demonstrates how to do the following:

1. set up a transient bubble column
2. use the Eulerian multiphase model
3. solve the problem using appropriate solver settings
4. postprocess the resulting data

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1 Introduction

1.1 Bubble column technology

Bubble columns are multiphase reactors where a gas phase is dispersed into a continuous phase (i.e., a liquid phase—two-phase bubble column: the subject of this study—or a suspension—slurry bubble column) in the form of “non-coalescence-induced”/disperse bubbles or of “coalescence-induced” bubbles. The two-phases are separated by an interface between the dispersed phase and the continuous phase; at this interface, interfacial transport phenomena (i.e., heat and mass transfer) may occur.

Two-phase bubble columns are widely used in chemical, petrochemical and biochemical industries thanks to the many advantages they provide in both design and operation. They are used, for example, in the Fischer-Tropsch process for the production of liquid hydrocarbons and in the *LOPROX* process which aims to improve the biodegradability of heavily contaminated production effluents (e.g., containing organic substances, i.e., phenol) before they are transferred to the traditional biological wastewater treatment facilities (Degaleesan et al. (2001), Besagni (2021a)). They are also employed in nuclear reactors to remove radioactive particles from a contaminated gas flow. This is generally referred to as pool scrubbing.

On the practical point of view, the simplicity of construction, the lack of any mechanically operated parts, the low energy input requirements, the large contact area between the liquid and gas phases, and the good mixing within the liquid phase are some of the practical advantages in bubble column technology. The simplest bubble column configuration consists in a vertical cylinder with no internals, in which the gas phase enters at the bottom—through a gas sparger—and the liquid phase is supplied in batch mode (Figure 1) or it may be led in either co-currently or counter-currently to the upward gas stream.

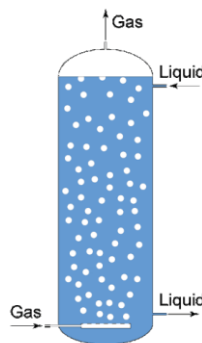



Figure 1: Layout of a bubble column.

Eventually, internal devices may be added to control the heat transfer, to limit the liquid phase back-mixing or to foster the bubble break-up rate. These elements have significant effects on the fluid dynamics inside the reactor and the prediction of these effects is still hardly possible without experimentation. It is worth nothing that the mass transfer that takes place at the interface does not necessarily involve reactions between gas and liquid components, even if this occurs in many practical cases. Despite the simple bubble column design, complex fluid dynamics interactions and coupling

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between the phases (which manifests in the prevailing flow regimes) exist; please note the fluid dynamics in bubble columns is similar to the ones observed in nuclear and energy conversion systems. Therefore, correct design and operation of bubble column reactors rely on the proper prediction of the global and local fluid dynamic properties: a typical approach is apply scale-up methods to estimate the fluid dynamics of “industrial-reactor-scale” reactors from “laboratory-reactor-scale” experimental facilities (Figure 2). Subsequently, models for the interfacial mass transfer and, eventually, to take into account the multi-phase reactions, are applied. Among the many fluid dynamic properties, the gas holdup (ε_G)—a dimensionless parameter defined as the volume of the gas phase divided by the total volume of the system—is a global fluid dynamic property of fundamental and practical importance. The gas holdup determines the mean residence time of the dispersed phase and, in combination with the size distribution of the dispersed phase, the interfacial area for the rate of interfacial heat and mass transfer.

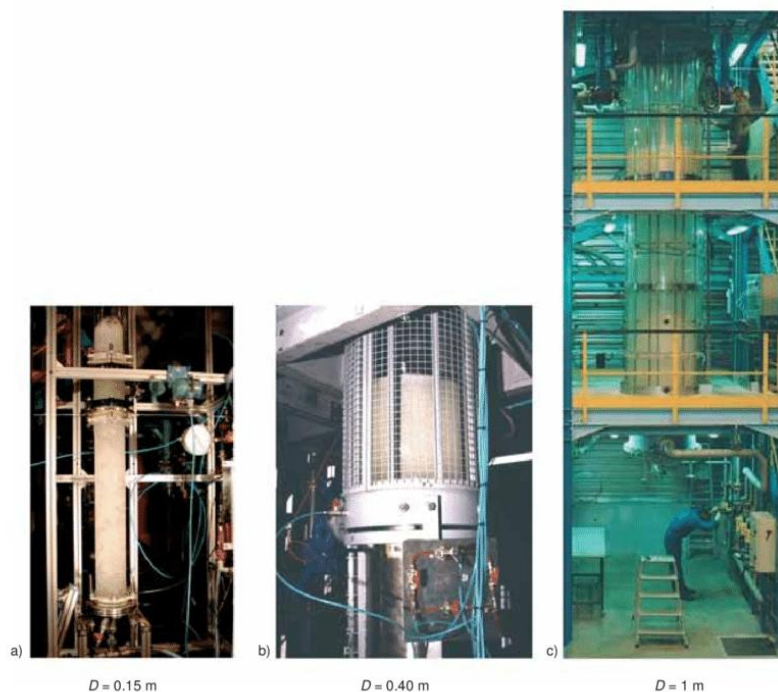



Figure 2: Example of bubble columns.

1.2 Flow regimes in bubble columns

The global and the local fluid dynamic properties depend on the many variables of the systems (i.e., the operation mode, the physical properties of the phases, the properties at the gas-liquid interface, ...) and are related to the prevailing flow regime.

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In the most general case, as the superficial gas velocity is increased, four flow patterns can be encountered in vertical pipes: (1) homogeneous regime, (2) slug flow regime, (3) heterogeneous (churn-turbulent) regime, and (4) annular flow regime (Figure 2).

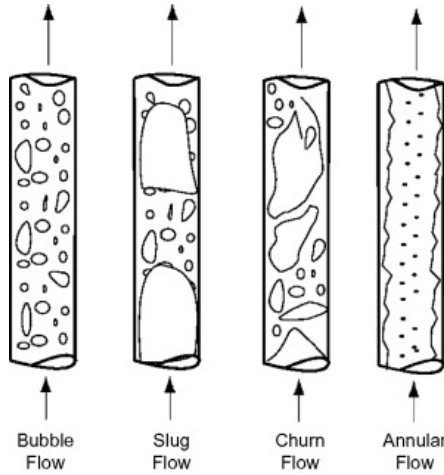


Figure 2: Flow regimes in vertical pipes.

When going towards industrial applications, large diameter systems has to be considered. The definition of large-diameter bubble columns is related to the fluid dynamics properties and, in particular, to the absence of the slug flow, resulting from Rayleigh-Taylor instabilities. The quantification of these instabilities at the reactor scale is obtained by comparing the non-dimensional diameter, D_H^* , with a critical diameter, $D_{H,cr}^*$:

$$D_H^* = \frac{D_H}{\sqrt{\sigma/g(\rho_L - \rho_G)}} > D_{H,cr}^* = 52 \quad (1)$$


In Equation (1) D_H is the hydraulic diameter of the bubble column, σ is the surface tension, g is the acceleration due to gravity, and $\rho_L - \rho_G$ is the density difference between the phases. A bubble column is classified as a large-diameter column if D_H^* is greater than $D_{H,cr}^* = 52$ (Brooks et al., 2012).

Under the constrain of Equation (1) the fluid-dynamics of large-diameter bubble columns explicates in six flow regimes and is interpreted by a function of two global fluid dynamics parameters, the drift flux and the gas holdup. The analytical relation between J_T and ε_G builds on five flow regime transitions points (Figure (3)).

The drift flux is defined as the volumetric flux of either components relative to a surface moving ing at volumetric average velocity expressed as follows:

$$J_T = U_G(1 - \varepsilon_G) \pm U_L \varepsilon_G \quad (2)$$

The sign on the right and side of Equation (2) depends on the bubble column operating mode: co-current mode (+) or counter current mode (-); in the batch mode $U_L = 0$.

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The six flow regimes emerging upon an increase in the gas flow rate, at fixed system design parameters, phase properties, and operating modes are as follows. First, the “*mono-dispersed homogeneous*” and “*poly-dispersed homogeneous*” flow regimes are progressively observed. The former, is characterized by a mono-dispersed bubble size distribution, by the latter by a poly-dispersed one, according to the change in sign of the lift coefficient. Then the transition flow regime (named transition flow regime without coalescence-induced structures) begin to be established, by non-stable “*coalescence-induced*” structures, which induce gas holdup oscillations. Subsequently, “*coalescence-induced*” structures become stable, thereby characterizing the transition flow regime with coalescence-induced structures. Despite “*coalescence-induced*” begin present in the bubble column they are not completely developed. Indeed, increasing the gas flow rate resulted in a decrease in the gas holdup, thus unveiling the imbalance between higher gas flow rate and the formation of “*coalescence-induced*” structures, which are a clear indication of a transition process from prevailing fluid dynamics. Finally, stable coalescence-induced structures emerge, and the “*pseudo-heterogeneous*” and “*pure-heterogeneous*” flow regimes take place.

The former is characterized by an equilibrium between the increase in the flow rate (in terms of the drift flux) and the formation of “*coalescence-induced*” structures. This ends in a constant gas holdup for different drift flux values and is an indication that “*coalescence induced*” structures are well established. Conversely, in the “*pure-heterogeneous*” flow regime, increasing the gas flow rate increases the contribution of “*coalescence-induced*” structures. For this reason, in this particular flow regime, the influence of the initial boundary condition is lost.

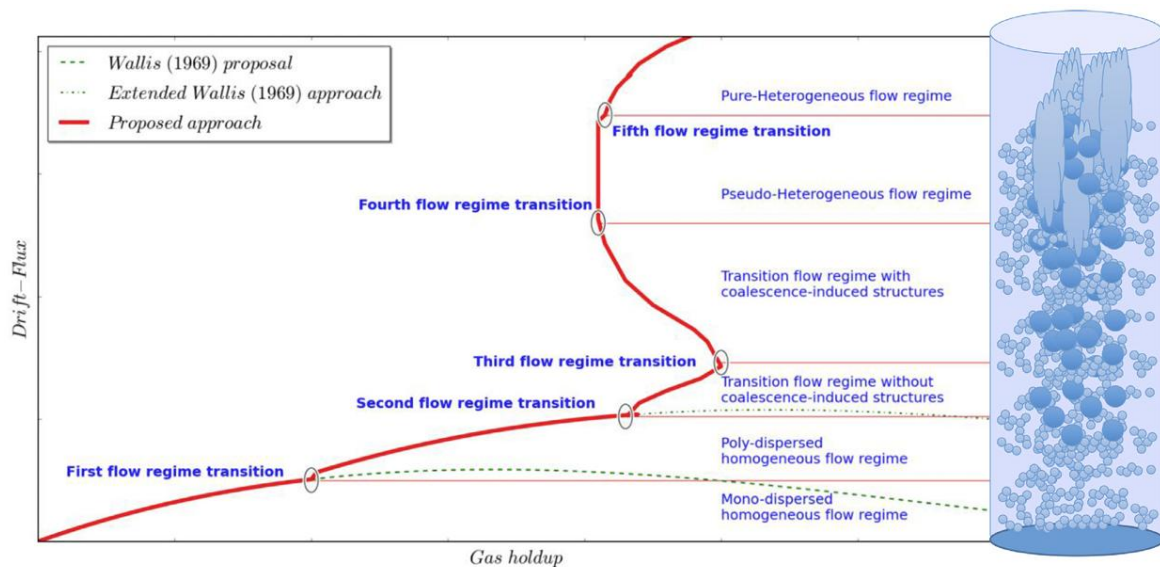



Figure 3: Bubble column characteristic curve.

1.3 Problem description

Air is injected at $U_G = 0.009673$ m/s (experimental value) ≈ 0.01 m/s into a rectangular-cross section (1 m x 0.10 m x 0.02 m) bubble column by a porous gas sparger (ensuring a mono-dispersed bubble size distribution having a mono dispersed BSD, provided as material in this class. You are requested to:

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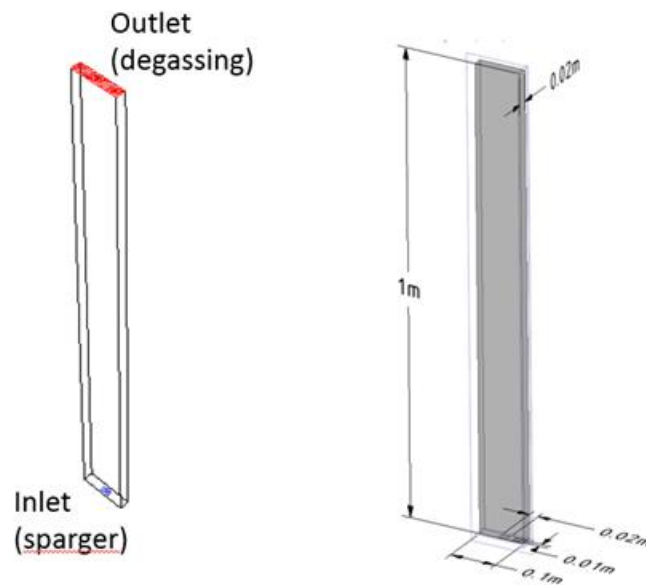
1. evaluate the gas holdup;
2. evaluate the interfacial area;
3. observe and analyze the disperse phase dynamics;

2 Simulation of the bubble column fluid dynamics

2.1 Preparation

Perform the following preliminary steps:

- Analyze the engineering problem
- Check the mesh




The 3-D case file (bub-col.cas.h5) is available.

Note. A very coarse mesh has been used in order to allow the transient simulation to be completed within a reasonable time. A mesh refinement study would likely show that a mesh independent solution would not be obtained for this problem with the current mesh resolution.

2.2 Solver settings

Bubble columns are characterized by a transient and density-driven fluid dynamics

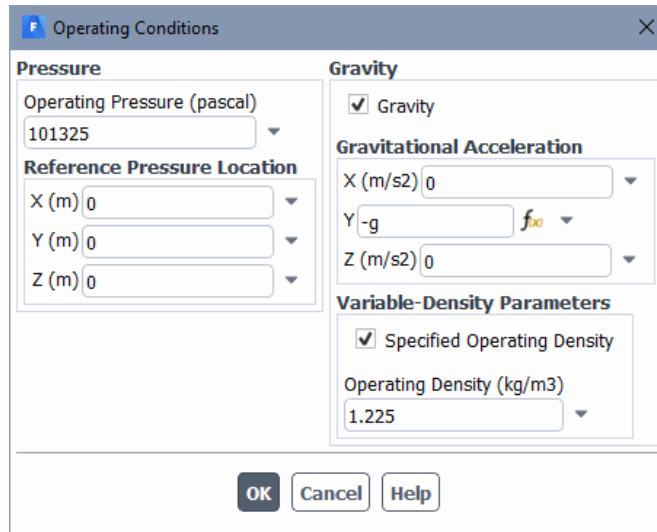
Physics tab → Solver group

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Select transient on the task page.

Physics tab → Solver group → Operating Conditions

Set gravity and enter an expression of $-g$ (or 9.1 m/s^2) for the gravitational acceleration in the Y direction. Also set operating density equal to the one of the lighter phase (1.225 kg/m^3).



2.3 Multiphase model settings

We have to solve a monodispersed homogeneous flow regime (with two phases) using the Eulerian multiphase model.

Physics tab → Models group → Multiphase


Select Eulerian model and specify 2 phases.

Physics tab → Materials → Create/Edit

Air and water are needed as the two phases to be modelled. Thus, in the fluent database materials dialog box select water-liquid and copy it (retain the default property values).

Physics tab → Models group → Viscous

Select $k-\omega$ SST dispersed model. The dispersed turbulence model is an appropriate model when there is clearly one primary continuous phase and the concentrations of the secondary phases are dilute. The random motion of the secondary phases is influenced by the primary- phase turbulence. Please note that for these cases a Per phase model would be suitable as well.

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Multiphase Model

Models

Phases

Phase Interaction

Population Balance Model

Model

☐ Off

Homogeneous Models:

☐ Volume of Fluid

☐ Mixture

☐ Wet Steam

Inhomogeneous Models:

☒ Eulerian

Number of Eulerian Phases

2

Regime Transition Modeling

☐ Algebraic Interfacial Area Density (AIAD)

☐ Generalized Two Phase Flow (GENTOP)

Eulerian Parameters

☐ Dense Discrete Phase Model

☐ Boiling Model

☐ Multi-Fluid VOF Model

Volume Fraction Parameters

Formulation

☐ Explicit

☒ Implicit

Apply

Close

Help

Viscous Model

Model

☐ Laminar

☐ k-epsilon (2 eqn)

☒ k-omega (2 eqn)

☐ Reynolds Stress (7 eqn)

k-omega Model

☐ Standard

☐ GEKO

☐ BSL

☒ SST

k-omega Options

☐ Low-Re Corrections

Options

☐ Curvature Correction

☐ Production Kato-Launder

☒ Production Limiter

Turbulence Multiphase Model

☐ Mixture

☒ Dispersed

☐ Per Phase

Model Constants

Alpha*_inf

1

Alpha_inf

0.52

Beta*_inf

0.09

a1

0.31

Beta_i (Inner)

User-Defined Functions

Turbulent Viscosity

phase-1

none

phase-2

none

OK

Cancel

Help

Physics tab → Models group → Multiphase

In the phases tab rename the primary phase water and set the phase material to water-liquid. Rename the secondary phase air.

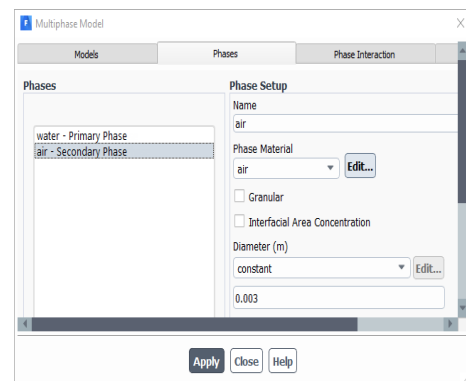
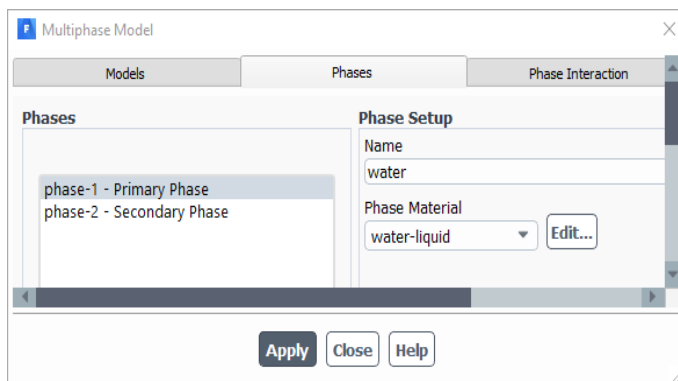
The equivalent diameter of bubbles at the inlet are set according to experimental digital image analyses. When experimental bubble size distributions (BSD) are available (as provided as material in this class), they can be analyzed and plotted using N-bins and, then, average diameter of each can be calculated using the as follow:

$$d_b = \frac{\sum_{i=1}^N n_i d_{b,i}^3}{\sum_{i=1}^N n_i d_{b,i}^2} \quad (1)$$

where $d_{b,i}$ and n_i are the diameter and the number of bubbles of size class i , respectively, and N is the number of size classes in the BSD.

Set the interactions:

- Universal-drag for drag coefficient
- Tomiyama for the lift coefficient
- Antal-et-al for wall lubrication
- Burns-et-al for turbulent dispersion
- Sato for turbulent interaction
- Surface tension = 0.072 N/m




2.3.1 Boundary condition settings

Physics tab → Zones group → Boundaries -> inlet

Select mixture from the phase drop-down list and click edit; select normal to boundary from the direction specification method drop-down list.

Select water from the phase drop-down list and click edit; enter 0 kg/s for mass flow rate.

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Select air from the phase drop-down list and click Edit; enter the suitable value for the mass flow rate. From the slip velocity specification method select volume fraction from the drop-down list. Enter 1 for volume fraction.

Retain default settings for turbulent quantities.

Physics tab → Zones group → Boundaries → Outlet

Select mixture from the phase drop-down list. Select degassing from the type drop-down list to change from a pressure-outlet to a degassing boundary. Degassing boundary condition allows the secondary phase to exit and behaves like a free slip surface for the primary phase.

Physics tab → Zones group → Boundaries → Wall

At the walls, a no-slip boundary condition is applied for the continuous phase and a free-slip condition is assigned for the disperse phase.

2.4 Solution method settings

Solution tab → Solution group → Solution controls


Retain the default settings for solution controls.

Solution tab → Solution group → Methods

Select PRESTO! for Pressure, Second Order for Momentum, Modified HRIC for Volume Fraction, from the drop-down lists under Spatial Discretization. Bounded Second Order Implicit from the Transient Formulation.

Solutions tab → Reports group → Residuals

Suggested iterations to plot = 100. It is generally suggested to have 20 iterations per time step of, ensuring maximum residual values below 10^{-5} for all equations.

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The screenshot shows the 'Task Page' window with the following settings:


- Solution Methods** (with a help icon):
 - Pressure-Velocity Coupling**:
 - Scheme: Phase Coupled SIMPLE (dropdown)
 - ☐ Solve N-Phase Volume Fraction Equations
 - Spatial Discretization**:
 - Gradient: Least Squares Cell Based (dropdown)
 - Pressure: PRESTO! (dropdown)
 - Momentum: Second Order Upwind (dropdown)
 - Volume Fraction: Modified HRIC (dropdown)
 - Turbulent Kinetic Energy: First Order Upwind (dropdown)
 - Specific Dissipation Rate: (dropdown)
 - Transient Formulation**:
 - Bounded Second Order Implicit (dropdown)
 - ☐ Non-Iterative Time Advancement
 - ☐ Frozen Flux Formulation
 - ☐ Warped-Face Gradient Correction
 - ☐ High Order Term Relaxation (with an 'Options...' button)
 - Default (button)

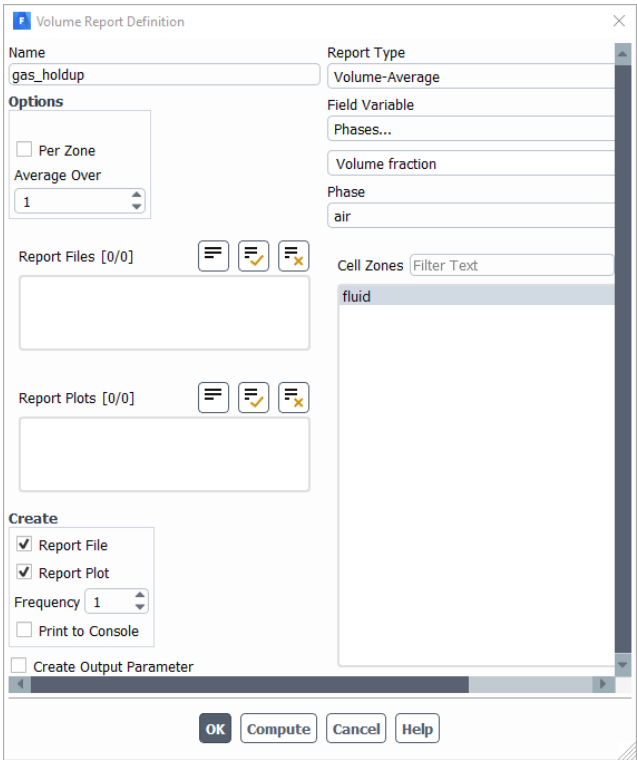
2.5 Report settings

Reports and graphics are intended to provide insights in the global and local flow phenomena.

Report tab → New > Volume Report of type Volume- Average

Enter gas holdup for name. Enable report file and report plot. Select phases and volume fraction from the variable drop-down list and search for air. In the list of cell zones select fluid.

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Surface tab → Create → Surfaces → Iso-Surface

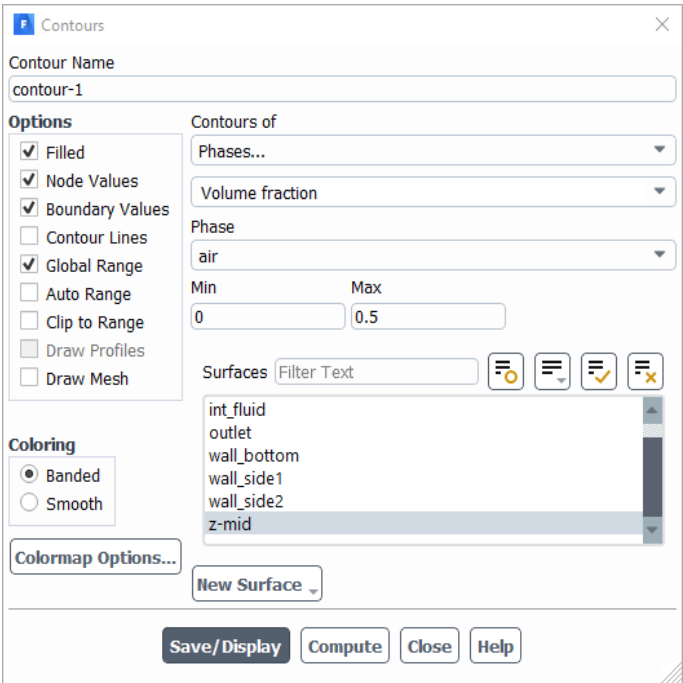
In the Iso-Surface dialog box, select mesh and Z-Coordinate from the surface of constant dropdown lists. Enter 0.01 for Iso-Values. Enter z-mid for new surface name. To activate this tab you need to initialize the solution. In the Solution Initialization task page, select inlet on the Compute from drop-down list. Click Initialize.

Graphics tab → Mesh → New

In the mesh display dialog box, select only faces in the options group box. From the list under surfaces select only wall_side1 and wall_side_2. Click Save/Display and close the Mesh/Display dialog box. Similarly create another mesh object, selecting the zones inlet and wall_bottom, while keeping both faces and edges enabled

Graphics tab → Contours → New

Enable filled under options. Disable auto range and clip to range. Select Phases and Volume fraction from the. Contours of drop-down lists. Select air from the Phase drop-down list. Enter 0 for Min and 0.5 for Max. From the list under Surfaces select z-mid. Click Save/Display and close the Contours dialog box.



Results → Scene → New

In the Scene dialog box that opens, under Graphics select the check boxes for contour-1, mesh-1 and mesh-2.

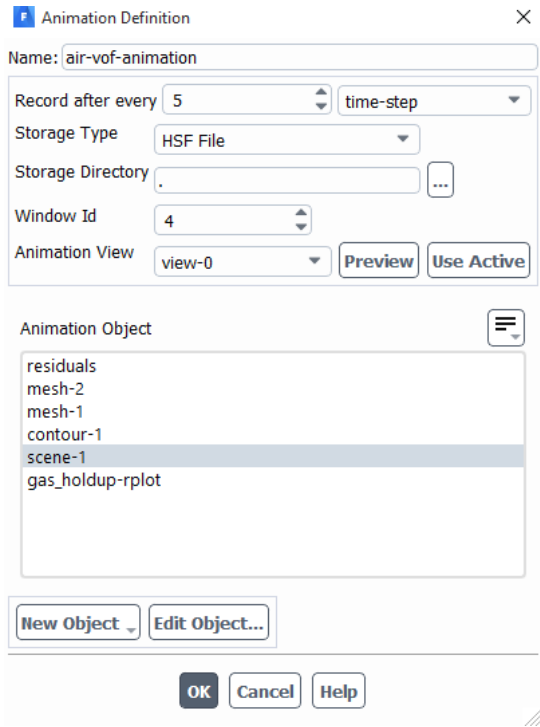
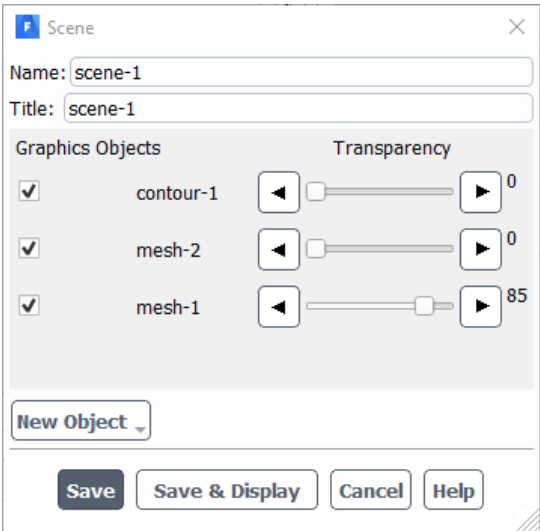
Note: Mesh-1 is the mesh object with wall_side1 and wall_side2. The transparency does not have to be the exact value, just something close. You can experiment with other values to find what you think has the best appearance. Click Save & Display and then you can close the Scene dialog box.

Solution tab → Activities group → Autosave .

In the Autosave dialog box, enter 250 for Save Data File Every (Time Steps).

Solution tab → Activities group → Create → Solution Animations

Rename the animation object to air-volume-fraction animation; Enter 5 for record after every; Select scene-1 from the list under Animation Object; Re-orient the view as desired and click on Use Active



2.6 Initialization and calculation settings

Solution Initialization task page

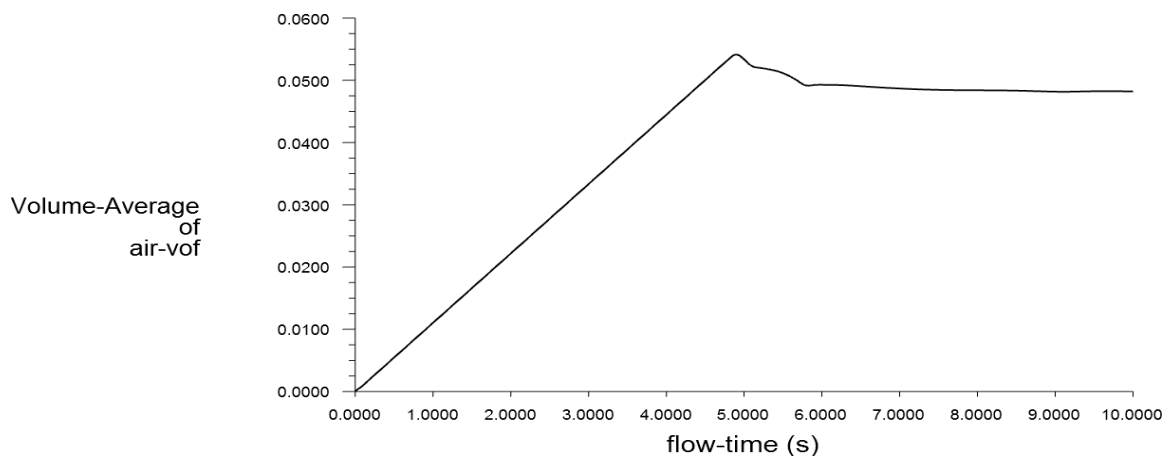
The column is initially filled with water, as in experiments, and null velocities are set. Click Initialize. Save the case and data files as bub_col.cas.h5

Run task page

In the run Calculation task page, enter 0.02 s for time step size (20 iterations for time step). Also, enter 500 for number of time steps.

2.7 Post-processing

Gas holdup. Gas holdup is the volume fraction of gas in the total volume of gas–liquid phase in the bubble column, which is one of the most important parameters to characterize the hydrodynamic characteristics of the bubble column. The plot from shows the initial transient startup behavior of the flow has begun to stabilize (approximately 4.7 %).




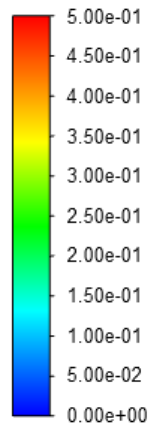
Interfacial area. It can be computed based on $a_i = 6 \frac{\varepsilon_G}{d_{23}} \left[\frac{1}{mm} \right] \rightarrow \frac{6}{3mm} \varepsilon_G = 2 \varepsilon_G \left[\frac{1}{mm} \right] = 0.094 \left[\frac{1}{mm} \right]$. In practical applications, a large contact area between the phases ensures high interfacial heat and mass transfer and, eventually, high reaction rate.

Flow phenomena. You can check the contours in the window of contours of gas holdup (volume fraction of air) as well as the gas holdup evolution over time.

Results tab → Animation group → Solution Playback

In the playback dialog box, select animation-1 from the list under animation sequences.


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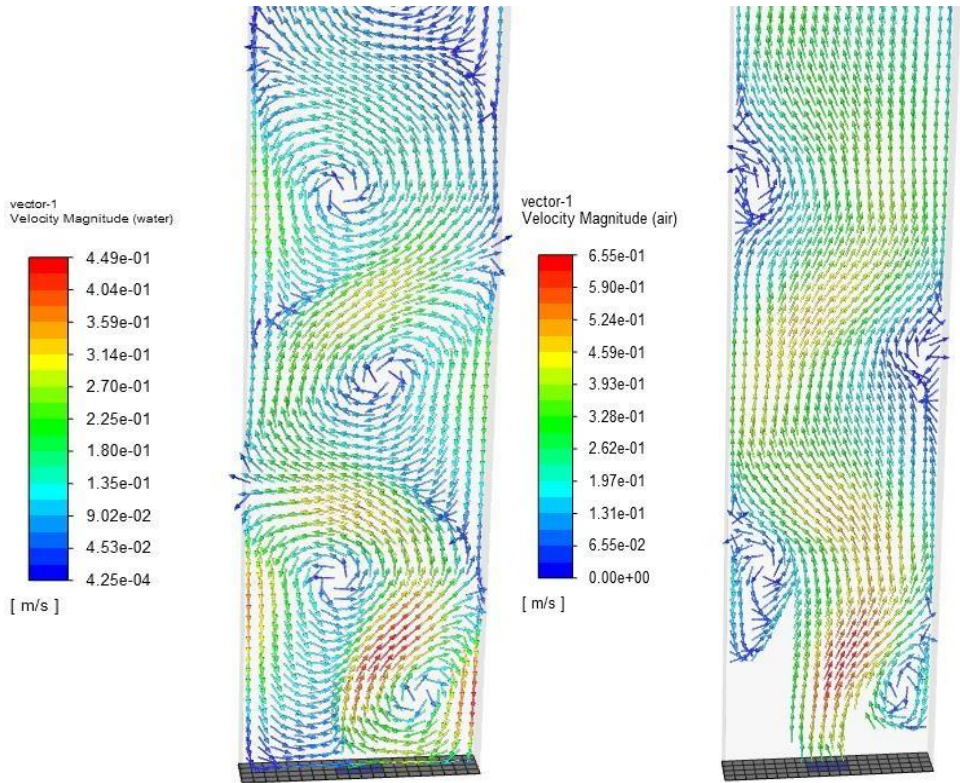
contour-1
Volume fraction (air)

You can check the contours in the window of contours of gas holdup (volume fraction of air) as well as the gas holdup evolution over time. After a certain period, the oscillatory motion of the bubble plume is restricted to the lower part, while in the upper part the gas volume fraction distribution is more uniformly distributed. This has to be attributed to the developing flow field and acting bubble lift and turbulent dispersion forces. The transient nature of this flow with a lower oscillating region and a more uniform region in the upper part was nicely captured by the model.

Create → Vector

Select water from the Phase drop-down list; Select z-mid from the list of surfaces. Depending on the vector style, it may be helpful to reduce the value in the scale field. Select air from the phase drop-down list; select z-mid from the list of surfaces. You may click Save/Display at the different steps

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3 Assignments

1. There is an initial transient period and it is usually desirable to begin the time averaging only after the effects of the initial transient have faded.

Run -> Data sampling for time statistics

Time averaging will be performed for another 10 seconds and the time averaged profile of the air will be plotted on a cross section 0.2 m above the bottom of the column.

Create -> Surfaces -> Iso-Surfaces

In the Iso-Surface dialog box, select mesh and Y-Coordinate from the surface of constant dropdown lists; Enter 0.2 for Iso-Values; Enter y=0.2m for new surface Name; select z-mid from the list under from surface;


Results tab -> Plots group -> XY Plot -> New

Enter vof-at- y=0.2m for name. Retain the values of 1,0,0 for X,Y, and Z respectively under plot direction. Select air from the phase drop-down list. Select unsteady statistics and mean volume fraction from the Y Axis function drop-down lists. Select y=0.2m from the list of surfaces. Use the axes setup panel to provide a fixed maximum value of 0.16 under the plot range

Solution tab -> Activities group -> Create -> Solution Animations

Enter gas-plot-animation for Name; Enter 5 for Record after every time steps; Select vof-at-y=0.2m from the list under Animation Object

2. Check the influence of the drag force (i.e., Tomiyama drag force and Grace drag force); What happens? Why?
3. Change the bubble diameter to 4 mm

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