High fidelity simulations of Taylor bubbles in turbulent co-current flow

by

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1 Introduction

1.1. Introduction to Computational Fluid Dynamics

Since the 19$^{\text{th}}$-century significant efforts have been made in the field of fluid dynamics to understand the physical behavior, motion, and properties of fluids to translate them into mathematical expressions and governing laws.

The basic governing equations representing the flow of a viscous fluid are the Navier-Stokes equations which were derived from the application of Newton's second law of motion to fluid motion and are also called momentum equations. The Navier-stokes equations are extensions of the Euler Equations and include the effects of viscosity [1]. In the case of Newtonian fluid, the conservation form of Navier-Stokes momentum equations describe a balance between inertia, pressure, viscosity and external forces and is given in differential form by

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \frac{1}{3} \mu \nabla (\nabla \cdot \mathbf{u}) + \rho \mathbf{g}, \tag{1.1}$$

where ρ is the fluid density, u the velocity field of the fluid, t the time, p the pressure, μ the dynamic viscosity and g the gravitational acceleration when gravity is the external force [1]. In particular:

- $\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u})$ indicates the momentum convection,
- $-\nabla p$ demonstrates the pressure,
- $\mu \nabla^2 \mathbf{u} + \frac{1}{3} \mu \nabla (\nabla \cdot \mathbf{u})$ displays the viscous forces,
- and the last term $\rho \mathbf{g}$ the external(i.e. gravitational) forces.

If we rewrite the Navier-stokes into dimensionless form, a very important dimensionless quantity will come from the viscous and convection terms, known as Reynolds number. The Reynolds number comprises the most important dimensionless number in fluid dynamics because it characterizes the flow and is defined as the ratio of inertial over viscous forces according to the formula

$$Re = \frac{\rho U L}{\mu} = \frac{U L}{\nu}, \tag{1.2}$$

where ν is the kinematic viscosity, L is the characteristic length, and U the upstream velocity. If $Re >> 1$, then inertia forces dominate while in case of $Re << 1$ friction forces (i.e. viscosity) dominate [2].

The Navier-Stokes equations are always solved together with the continuity equation which is known as conservation of mass as well as a particular set of boundary conditions. Together they form a boundary value problem [1]. The conservation of mass is described by the continuity equation and is given in differential form by

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{1.3}$$

Navier-Stokes equations are usually too complex to be solved analytically, except for a few simple cases [1]. Therefore, a numerical approach is needed to be able to solve them. During a numerical approach, the first step is the spatial discretization of a domain, known as mesh generation. Depending on the problem, the Navier-Stokes equations can be solved either iteratively or directly.

The choice of spatial discretization method is very important for achieving accurate calculations. The typical discretization methods are finite difference, finite element, and finite volume methods. The common idea in all methods is to divide the geometrical domain into very small finite parts (i.e. mesh generation). There are three types of grids: structured grids, unstructured grids, and block-structured grids [2],[3].

The Navier-stokes equations are unsteady in their general form and they need to be discretized also in time. In general, the temporal discretization is done through integration over time on the discretized equation. Temporal discretization methods varies in numerical analysis from fully implicit to fully explicit methods depending on the number of the weighted average between current and future values. Implicit methods are computationally more expensive and sometimes they can be much harder to be implemented than explicit methods. However, implicit methods may achieve fast convergence rates and they are preferred when stability plays an important role e.g. at stiff problems [4], [2], [3].

Runge-Kutta methods are a family of both implicit and explicit iterative methods that are widely used in numerical analysis for the solution of Navier-Stokes equations. The solvers of Navier-stokes equations can be also divided to coupled solvers where velocity and pressure are solved simultaneously (e.g. backwards differencing schemes, Crank-Nicolson scheme) or segregated/splitting methods where the velocity and pressure are solved sequentially (e.g. SIMPLE, PISO).The selection of the appropriate temporal discretization methods depend on the computational cost and the required stability [3], [2].

High-speed computers have been used for the implementation of numerical solution to Navier-stokes equations. The accuracy is determined by the choice of the spatial and time discretization scheme, the stopping criterion selected by the user, or simply by the floating-point precision of the system used. The simulation results of a problem are compared with the results derived from experiments and possible errors are determined. This is an iterative process until the maximum accuracy is achieved. The whole process is illustrated in figure 1.1.

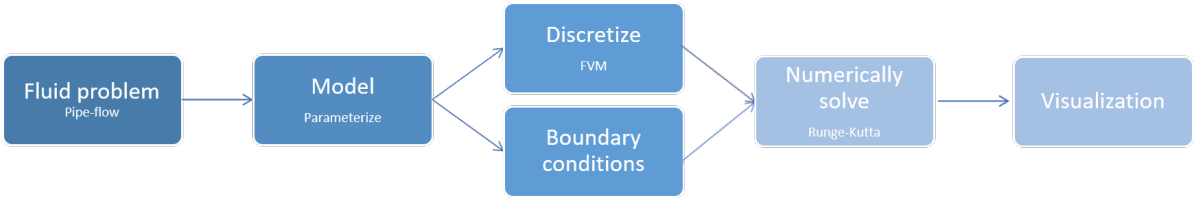

Figure 1.1: Flow chart of the CFD process in a fluid problem

This process is defined as Computational Fluid Dynamics, or CFD for short. This makes CFD a crossing point of three disciplines: Fluid dynamics, Mathematics, and Computer science, as it numerically solves complex partial differential equations to describe the behavior of fluids [5].

There are many high-performance CFD software packages. Their main division is between commercial and open-source software packages. Open-source means that the user is free to view and modify the underlying code of the software. Both open-source and commercial CFD software packages are used in a wide range of research and industrial areas. CFD is a great research, educational and industrial tool which covers the fields of aerospace, automotive engineering, chemical and mineral processing, biomedical science, civil and environmental engineering as well as power generation [5].

1.2. Multiphase Flows

A fluid flow can be characterized as:

- laminar or turbulent flow depending on the value of Reynolds number, and
- single-phase fluid flow or Multi-phase fluid flow depending on the number of phases that simultaneously exist.

Classic study of fluid dynamics is focused on the flow of a single homogeneous phase such as water, air or steam [6]. In cases and locations where the fluid flow consists of more than one state or component,

the relatively simple relationships used for analyzing single-phase flow are insufficient and the problem must be solved as multiphase flow [7].

Multiphase flow is defined as the simultaneous flow of materials with two or more different thermodynamic states or phases (e.g. steam-water flows)[6]. Multiphase flow takes also place when there are two or more materials with different physical properties but in the same phase or state (e.g. oil-water flows) [8]. Therefore, in the second definition the word "multi" is referred to the different components and not to the amount of "phases" even though this kind of flows is also called multiphase. Every phase of each material depicts a volume fraction of solid, liquid or gaseous matter with its properties such as velocity and temperature [6]. In cases where the temperature of one phase is different from the temperature of the other(s) state(s), then there is also multiphase heat transfer through their interfaces. Moreover, if the heat transfer takes place between different phases of the same material, then the heat transfer is also followed by mass transfer (solid-liquid, solid-vapor or liquid-vapor phase change) [9].

The analysis and solution of multi-phase fluid flow is usually very complex compared with conditions of single phase flow. The modeling of two-phase flow is still under development because there are many types of instabilities in multiphase flow.

The three main steps for the modelling of a multiphase flow problem consists the identification of the type of the multiphase flow, the specification of the physical process together with the phenomena may occur, and at the end the determination of the mathematical model [10].

First of all, it is essential to identify the characteristics of the flow and the important effects which will influence the choice of the appropriate model. This analysis requires the determination of the characteristics of the flow,the hydrodynamic effects as well as the transport phenomena. The characteristics of the flow consists the knowledge of the flow regime (e.g. bubbly flow,slug flow etc.), the grade of turbulence at the flow, the density and the viscosity of each phase, surface tension etc .Depending on the type of the flow, the hydrodynamic effects may include the change in interface,a particle-wall or particle-particle collision,a possible coalescence, turbulent flow etc. On the other hand, the transport phenomena may include heat transfer, mass transfer, change in composition or/ and heterogeneous reactions. Therefore the natural process specification may include the phenomena of separation, filtration, suspension, evaporation or reaction [11].

The specification of the flow regime between two or more immiscible fluids can be classified into types according to its behaviour. Three main types of the multiphase flow can be found in the literature [7], [9], [11]:

- Flow with separated phases: Different immiscible fluids in continuous phases which are separated by interface .
- Dispersed flow: Finite amount of components in dispersed phase (e.g. droplets, bubbles) which are spread within the volume of the other, continuous phase.
- Mixed Phases: Presence of both separated and dispersed phases .

Different examples of multiphase problems are classified with respect their phase type and are indicated at figure 1.2. Examples of flow regimes include discrete gaseous bubbles in a continuous liquid, discrete fluid droplets in a continuous gas/liquid , discrete solid particles in a continuous fluid (i.e. particle-laden), melting of binary solid, large bubbles in a continuous liquid (i.e. slug flow), continuous liquid along walls, gas in core (i.e. annular flow), immiscible fluids separated by a clearly-defined interface (i.e. stratified/free surface flows) [11].

The mathematical modelling of multiphase flows can be done with three ways:

- theoretically, through using governing equations and other mathematical formulas,
- experimentally, in fully- equipped laboratories, and
- using CFD packages by taking advantage of modern high-tech computers and their processors.

Due to the complexity of the flow in most engineering problems and the inability to apply Navier-Stokes equations for every phase and find the solution for every property at each single point of a multiphase flow, the predictions are based mainly on computational models and secondary on theoretical models. Testing experimentally can be very expensive for most of the problems and even impossible for others [7].

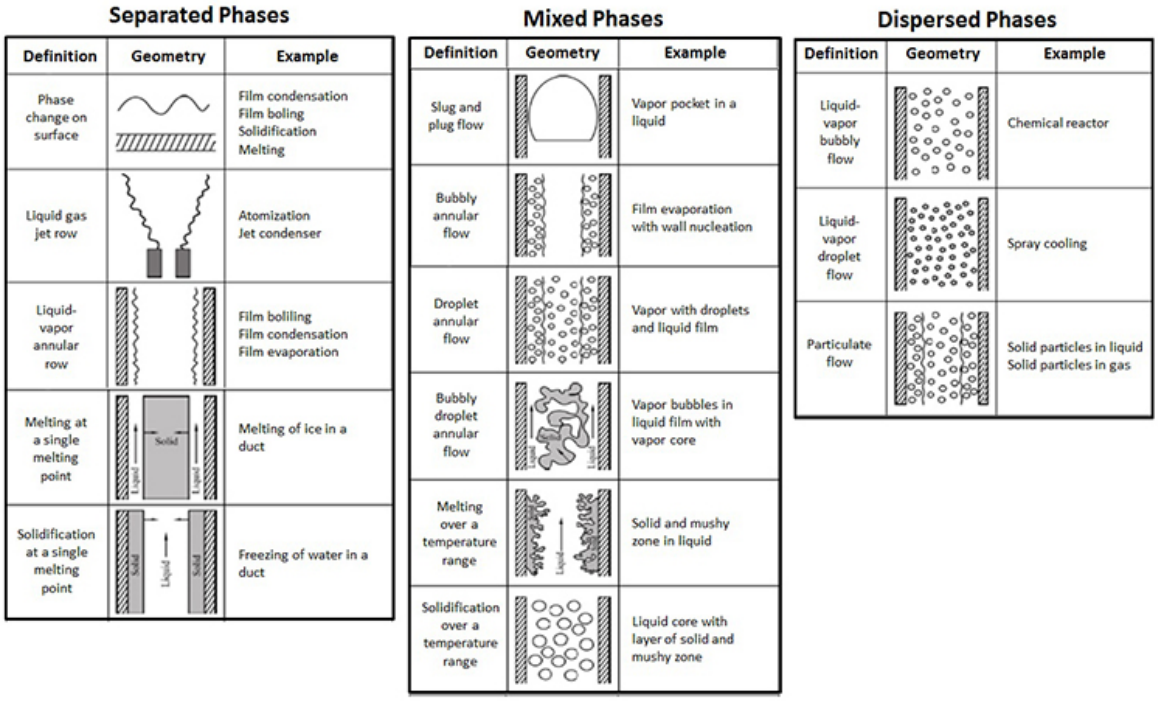

Figure 1.2: Multiphase flow regimes classified according to the type of phases as illustrated in [9].

In the case of multiphase flow with separated phases,the simplest approach for uncomplicated problems is to split the problem into different single-phase flows, apply the governing equations (Navier-stokes and mass conservation) to each of the phases and together with the relevant "jump conditions" at the interface, one can determine the solution [9].

However,the application of an interface analysis in multiphase flow problems with dispersed or mixed phases is impossible. At these cases, a control volume approach within the multiphase flow is usually followed with a space averaging of governing equations over all phases at the same time [9]. No matter which spatial discretization method is used, the volume fraction of each phase is given by the formula

$$\text{Volume of phase}_i = \frac{\text{Volume of the phase in the cell}_i}{\text{Total volume of the cell}}, \tag{1.4}$$

where $i \in [1, ..., n]$ indicates the referring phase in a n-phase flow.

Several mathematical models have been developed for the simulation of the multiphase flow depending on the physical process of the problem and the specification of the flow. The choice of the best model for each case is still a challenging decision. Generating both realistic and simpler models is the key factor for multiphase fluid flow simulations [7]. Two of the most popular mathematical modelling techniques for multiphase flows which are widely used in the literature are the Volume of Fluid(VoF) and the level set method (LS) [12], [13], [14]. Both of them belong under the umbrella of Eulerian front-capturing methods where the interface between the immiscible fluids is depicted as contact discontinuity on a fixed computational stationary mesh [12]. Except them, other commonly used mathematical approaches that can be found in the literature are [11]:

- Lagrangian Multiphase (LMP): Track individual point particles, particles do not interact e.g. in droplet flows.
- Discrete Element Method (DEM): Solve the trajectories of individual objects and their collisions, inside a continuous phase e.g. in particle flows.
- Eulerian Multiphase (EMO): Dispersed flow, particle flows, bubbly flows, boiling heat and mass transfers, interphase mass transfer.

- Eulerian/Lagrangian Dispersed Phase Model (DPM): Particle-wall interaction is always considered, particle-particle is usually not.
- Algebraic Slip Mixture Model (ASM): Neither particle-wall interaction nor particle-particle are considered.
- Eulerian-Eulerian Model (EEM): Particle-wall interaction is considered, particle-particle is usually not.
- Eulerian-Granular Model (EGM): Both particle-wall and particle-particle interactions are considered.
- Various empirical correlations.

Many real-world engineering problems rely on the numerical analysis of fluid flow, which typically consists of more than one phase. Multiphase regimes are taken place in automotive, oil and gas, power generation, paper, and pulp industry and even medicine. In particular, multiphase flow is important in many industrial processes such as fluidized bed in chemical reactors for emergency cooling, gas-liquid flows in evaporators and condensers in thermal power plants, bubbly flows in nuclear reactors, production of hydrocarbon in wells and their transportation in pipelines, pump cavitations, gas-particle flow in combustion reactors and fiber-suspension flows in paper and pulp industry [7], [8], [15], [13].

Last but not least, multiphase flow problems are also met in several natural phenomena. For instance, multiphase flow take place in sediment transport in river flow, withing clouds, at waves on the sea or between plasma and red blood cells in blood flow [7].

1.3. The case of Taylor bubbles rising in liquid flow

In pipe flow problems where both gas and liquid flow simultaneously, different multiphase flow regimes may arise (see figure 1.2) depending on the volumetric flow rates, the geometry (pipe diameter and length, wall roughness) and orientation of the pipe and several fluid properties (density, viscosity, surface tension) [16]. Among the resulting flow regimes, there is the case of slug flow where a disperse gas bubble is pushed along by a lighter and faster moving continuous fluid which contains gas bubbles [17]. Slug flow in a horizontal pipe is illustrated in figure 1.3.

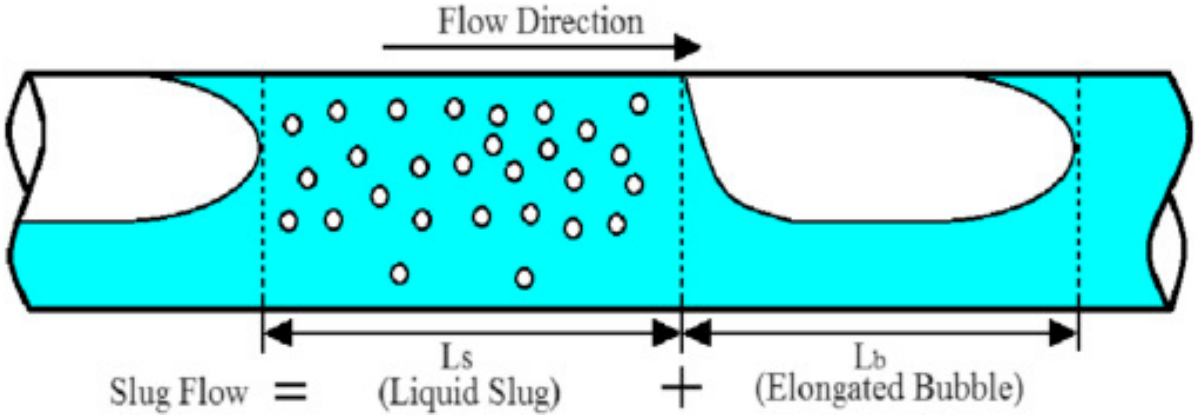

Figure 1.3: Flow regime of slug flow where gas bubbles push along a larger gas bubble in a liquid slug [18].

In the case of slug flow in a vertical pipe where gas is fed with different flow rates at the bottom of the pipe, the small gas bubbles follow a random distribution. The random movement of gas bubbles take place for any liquid velocity. The main difference is that the gravity acts along the pipe flow whereas in the horizontal pipe it was acting along it [12]. If the gas flow rate is further increased, the small bubbles are merging into a larger bubble, which is known as Taylor bubbles [16], [13].

Taylor bubbles are of bullet shape and occupying most of the pipe diameter and as the Taylor bubble's size is increasing, the thickness of the liquid film between the pipe wall and the bubble is becoming smaller. In real-world problems, Taylor bubble is often followed by other Taylor bubbles. The sequence of Taylor bubbles is separated by liquid slugs which consist of smaller dispersed bubbles[16].

Taylor bubble is moving along the pipe under the effect of gravitational, inertial, viscous and interfacial forces [13].

A very important parameter that influences the flow is the presence of the bubble wake behind the Taylor bubble. The possibility of the existence of the wake increases as the Taylor bubble is rising and the thin liquid film decreases. As it approaches the bottom of the pipe, the annular thin film moves downstream the Taylor bubble, within the area of liquid slug, and may create a wake. The possibility, the region and the order of magnitude the wake depends on the trailing edge of the Taylor bubble, the distance between two Taylor bubbles as well as on fluid properties(density, viscosity, surface tension, etc.), flow conditions (liquid and Taylor bubble velocity, temperature) and pipe geometry (wall roughness and pipe diameter and length) [16] .

Vertical gas-liquid slug flow with the creation of Taylor bubbles is met in many industrial processes such as in geothermal power plants, evaporation, and condensation in thermal power plants, oil extraction from wells, transportation of hydrocarbons through pipes and in the emergency core cooling of nuclear reactors [16], [13].

The main target of the current literature study is to illustrate the state-of-the-art numerical simulations and experimental results for the motion of the Taylor bubble within a pipe through background liquid flow and indicate the current scientific gap that can be explored through future work. Multiple databases were used for researching this literature study including Google Scholar, Sciencedirect, Web of Science, Scopus as well as the TU Library. The main sources were acquired by combining the search terms Computational Fluid Dynamics (CFD) and Taylor bubble flow.

The first chapter includes an introduction to Computational Fluid Dynamics and Multiphase Flows. The case of Taylor bubbles rising in liquid flow is introduced. In the second chapter, the most well-known mathematical modeling techniques are illustrated while in the third chapter, the accuracy and the limitations of software packages for the simulation of Taylor bubble flows are depicted. In the third chapter, results from numerical simulations that were found in the literature are presented and compared to each other with the experimental results. The analysis was implemented for stagnant, laminar and turbulent background liquid flows and both in two and three dimensions. In the last section, a discussion on the findings is illustrated followed by the research questions which the future work that will be done as the master thesis project will reply to.

2

Numerical Modeling Methods for the Simulation of Taylor Bubble Flow

The gas-liquid interface between Taylor bubble and the liquid within the pipe flow can be identified and controlled by using the appropriate numerical modeling method. The interface is non-stationary and its' form is changing in time. Therefore, a good numerical model provides the user the knowledge of gas-liquid interface's location and curvature at each time step. It is important to notice at this point that the choice of a numerical flow modeling technique is not a standalone flow solving algorithm. The governing equations describing the motion of the flow have to be solved separately like in all kinds of advection algorithms.

Significant efforts have been done for the numerical modeling of the Taylor bubble flow over the last decades. The different numerical techniques for multiphase flows can be characterized as either Eulerian front-capturing or front-tracking techniques. The main difference is that at Eulerian front-capturing techniques, the thin interface between gas-liquid on a fixed computational stationary mesh is interpreted as touch discontinuity and is implicitly specified by an indicator function while in the Eulerian front-tracking techniques, the interface is explicitly rebuilt.

Although there are some publications in which Eulerian front-tracking techniques are utilized for Taylor bubble flows ([19], [20], [21]) , the majority of the researchers are using front-capturing methods and therefore, this literature study will focus only on the latter [22], [23], [14], [24]. The most famous among them which can be found in the literature are the Volume of Fluid (VoF) and the level set method (LS). Both modeling techniques have some important disadvantages and for this reason many researchers have recently tried to define dual interface techniques which combine VoF and LS methods in order to minimize the drawbacks and increase solver's efficiency [12], [25].

2.1. Level-set method (LS)

The level set method is widespread among researchers for the simulation of Taylor bubble flows [26], [27], [28], [29]. The LS method provides an easy and implicit idea for the construction of the gas-liquid interface in the domain and it was first introduced at [30].

According to [31], the LS method is defined as " a particular family of transportation models in which a distance function (named level-set function) is transported". This distance function ϕ is an Eulerian function and is computed with respect to an interface, i.e. the interface (which is a surface in three-dimensions) is defined to be at the zero level set of the distance function. The distance function is a scalar quantity which is positive at the one phase (e.g. gas) and negative at the other phase(e.g. liquid) as shown in figure 2.1 obtained by [32]. The level set function ϕ is a signed scalar quantity which is advected by the moving fluid and can be applied to the transport equation [31], [28]:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0, \tag{2.1}$$

where u is the fluid velocity. The numerical solution of the level-set equation can be done with e.g. Finite-difference methods or upwind methods.

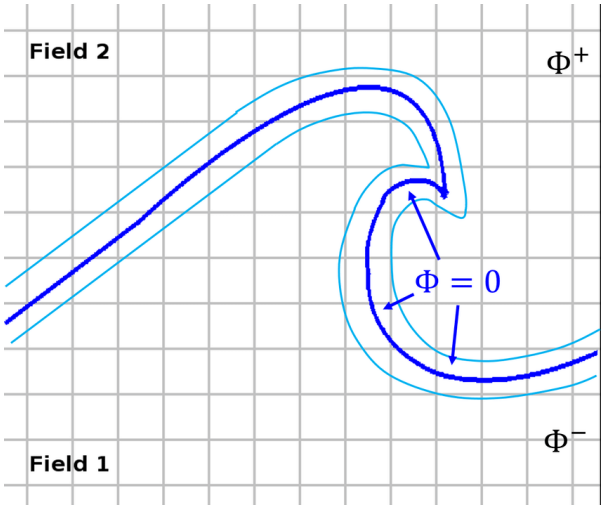

Figure 2.1: Schematic view of a Level-Set method on a moving interface, in green two isocontours of the Level-Set function Φ+ and Φ− are represented on each side of the interface as shown in [32].

Another important characteristic of the level-set function is that it should be an Eulerian function which means that the $||\nabla\phi|| = 1$. In Taylor bubble flows, the level set function ϕ may lose this property after some steps because of dissipation. As a consequence, it is necessary a re-initialization process should be applied every few iterations so that the Eulerian property is satisfied.

Unlike VoF method, any discontinuities near the interface at the values of the properties between gas and liquid would lead to stability issues. Therefore, at LS method it is essential to define a Heaviside kernel function $H(\phi)$ which usually is defined as:

$$\begin{cases} H(\phi) = 1 & \text{if} \quad \phi \geq 0, \\ H(\phi) = 0 & \text{if} \quad \phi < 0 \end{cases} \tag{2.2}$$

With the help of the smooth Heaviside kernel function, the material properties such as density and viscosity can be defined:

$$\rho(\phi) = H(\phi)\rho_g + (1 - H(\phi))\rho_l \tag{2.3}$$

$$\mu(\phi) = H(\phi)\mu_g + (1 - H(\phi))\mu_l, \tag{2.4}$$

where $\rho(\phi)$ represents the density with respect the distance from the interface, ρ_g the gas density, ρ_l the liquid density, μ the viscosity with respect the distance from the interface, μ_l the liquid viscosity and μ_g the gas viscosity.

Therefore, no matter how complex the multiphase flow is, the level set method can model easily the interface with the help of the smooth distance function even for sharp changes on fluid material properties. In some cases, due to the big differences of the velocity field, the distance function may show some deformations which lead to inaccurate results for the distance function in the areas far away from the interface. In order to fix this problem, some researchers tried to improve the accuracy by defining a correction function for re-distancing the level set contours [28]. Figure 2.2 indicates the results of the simulation of a rising bubble in a liquid domain using a conservative LS method [27]. This method decreases the problem of mass conservation of the standard level-set methods which was introduced by Balcázar at [33]. The idea of conservative LS method is the basis for the coupled/dual interfaces and it will be analyzed further later.

All in all, the LS method is relatively straightforward to be applied, computationally cheap and integrate smoothly complex topology changes. Therefore, it is easy to compute the mixture viscosity, density and surface tension. Moreover, the LS method shows good stability properties even for high gradients. However, the numerical implementation of interface advection with LS method is unable to preserve the volume of liquid and gas over time and therefore, although the individual phase volumes

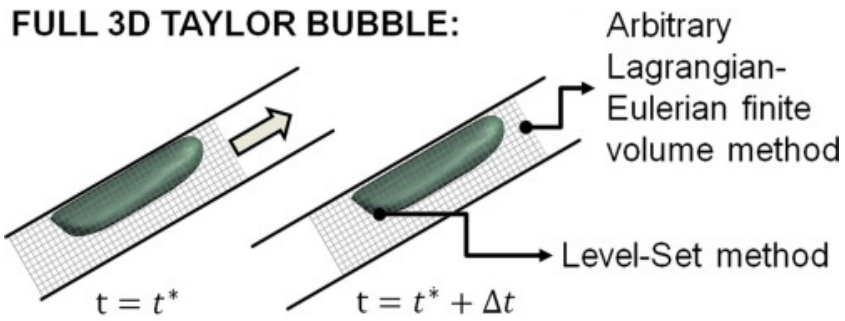

Figure 2.2: Simulation of a rising bubble which was implemented in [27] using conservative LS method as verified at [33].

may change over time, with the LS method they will remain constant due to the fact that conservation of ϕ does not imply conservation of mass [27].

2.2. Volume of Fluid (VoF)

Although the first publication of the VoF method was done four decades ago [14], the method still remains popular due to its' reliability and effectiveness and comprises the basis for the modeling of multiphase flows and in particular, of Taylor bubble flows. The VoF method, opposed to the LS method conserves the volume of the phases with time since the change of topology is implicit in the algorithm but it cannot give the specific position and curvature of the interface within a volume cell. As a consequence, the model needs more computations so that the user can identify the location of the interface and therefore, which leads to important CPU times. Therefore, VoF approach has in general more computational cost than LS method.

There are numerous publications simulating a Taylor bubble flow by using VoF method for the flow modeling [22], [23], [34], [35]. Many correction algorithms have been proposed for the improvement of efficiency and accuracy of the VoF method but the main idea is the same in all the cases.

After the mesh generation and the division of the domain into mesh cells, the idea of VoF method involves the definition of the volume fraction α. The volume fraction is a scalar function α which represents the quantity of gas (or liquid) in an individual computational mesh cell. It can be computed by

$$a_{i,j,k}h^3 = \int\int\int_{(i,j,k)} \chi(x,y,z)dxdydz, \tag{2.5}$$

where h is the mesh size and χ is the characteristic function of gas (or liquid) within the cell.

There are three different cases for the values of α in a single cell:

- α=1 , i.e. the cell consists only gas.
- α=0 ,i.e. the cell consists only liquid.
- $0< \alpha <1$, i.e. the thin gas-liquid interface passes through this cell. In this case, α is a discontinuous function and its' value jumps from 0 to 1 at some point within the cell. At the sudden increase of α from 0 to 1, the user can identify the direction perpendicular to the gas-liquid interface by using several approaches (Parker and Yong's method, finite difference method, Least-squares method etc.). In the three-dimensional case, the interface is represented by a plane while in two-dimensional case, it is just a line. However, the exact location and the curvature of the interface cannot be defined accurately and therefore, more local grid refinement has to be done which means more computational cost.

The volume fraction is applied in all cells for all time steps. The density and the viscosity of the fluid at each space point are not constant and their values are computed with the help of the volume fraction. When α=0, the density and viscosity at this space point (and at a specific time step) are given by the liquid's density and viscosity whereas when α=1, are given by the density and viscosity of the

gas. In the case where the interface is passing through a cell, the density and viscosity are computed by linear interpolation:

$$\rho = \alpha\rho_g + (1-\alpha)\rho_l \tag{2.6}$$

$$\mu = \alpha\mu_g + (1-\alpha)\mu_l, \tag{2.7}$$

where ρ represents the mixture density, ρ_g the gas density, ρ_l the liquid density, μ the mixture viscosity, μ_l the liquid viscosity and μ_g the gas viscosity [13].

The transport equation (or convection-diffusion equation) is a generalization of continuity equation and describes how a scalar quantity is transported in space [36]. Therefore, it can be applied to the volume fraction α after having an approximation for the interface. In the case of volume fraction, the transport equation should be solved without diffusion in order to eliminate smearing of the free-surface. Therefore the flux of α between mesh cells can be found by

$$\partial_t\alpha + \mathbf{u}\cdot\nabla\alpha = 0, \tag{2.8}$$

where $\mathbf{u}$ represents the mixture velocity which varies from cell to cell. The mixture velocity applied also to mass conservation (equation 1.3) the Navier-Stokes equations (equation 1.1) which now take the forms:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0, \tag{2.9}$$

$$\partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = -\nabla p + \rho\mathbf{g} + \nabla\cdot(2\mu D) + \sigma k\mathbf{n}\delta(n), \tag{2.10}$$

where μ and ρ are computed for each cell according to equations 2.6, 2.7, D illustrates the deformation tensor, σ surface tension, k the surface curvature, n the surface normal component, and interfacial Dirac delta function $\delta(n)$ .The last term in the right-hand side of Navier-Stokes equations represents the capillary term and is defined as the extra force applied onto the fluid because of the surface tension between gas and liquid and is non-zero only at the cells where $0 < \alpha < 1$, i.e. cells in which the gas-liquid interface is passing through. For incompressible flows the mass conservation equation 2.9 converts into $\nabla\cdot\mathbf{u} = 0$ [13].

The system of equations described before (equations 2.6 - 2.10) consists of seven equations for a three-dimensional Taylor bubble flow (since equations 2.10 gives one equation for each velocity component) with seven unknowns (ρ, μ, α, p, u_x, u_y, u_z) for each cell. In particular, a VoF algorithm solves the problem of updating in time the volume fraction α given the fixed mesh, the velocity field, the pressure distribution and the volume fraction α at the previous time step for all cells.

This means that the interface is rebuilt in each time step and the VoF method does not track the interface explicitly. The problem which occurs during the reconstruction of the interface in each time step, is that its' location and curvature should be approximated by knowing only the volume fraction of the cells from which the interface is passing (where $0 < \alpha < 1$) and their neighboring cells.

Several methods for the reconstruction of the interface exist, depending on the required accuracy and the computational cost and time. Among these, there are models with first-order accuracy where the reconstruction of the gas-liquid interface is done from a sequence of segments lined up with the grid cells. Most of the examples of first-order accuracy models are improvements on either the simple line interface calculation (SLIC) or the SOLA-VoF algorithm [37], [14], [38].

More accurate VoF techniques try to fit the interface through piecewise linear segments. One of the most widespread approach is the Piecewise Linear Interface Calculate (PLIC) [39]. The distinguishing feature of algorithms like PLIC is that they rebuilt the gas-liquid interface as a discontinuous (with asymptotically small discontinuities) and not as a continuous chain of segments as illustrated in 2.3. PLIC algorithm consists of a reconstruction and a propagation step. No matter how big is the curvature of the approximation of the interface, PLIC algorithm gives robust solutions and the discontinuities of interface's location may vary from $O(h^2)$ to $O(h^1)$ [38], [40], [41].

Moreover, there are also publications with high-order discretization schemes for the advective transport equation of multiphase flows which can also apply to Taylor bubble flows [42], [43]. All in all, the effectiveness and the accuracy of VoF method depends heavily on the choice of the discretization scheme used for the advection of the volume fraction.

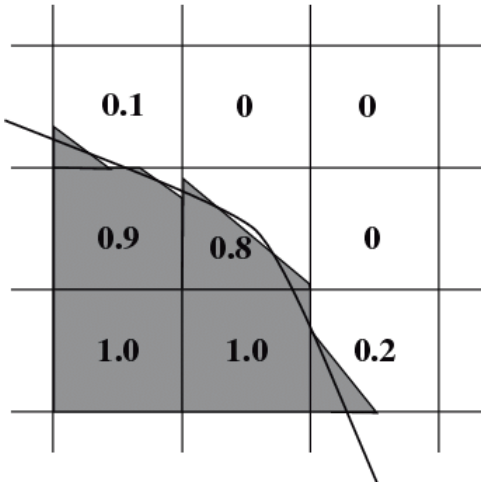

Figure 2.3: The basic principle of the VoF piecewise linear interface calculation (PLIC) method: the interface is reconstructed by linear unconnected segments in each cell [41].

2.3. Dual-interface methods

The bigger disadvantage of the LS method for the numerical modeling of interface advection in Taylor bubble flows is the lack of the conservation of volume of liquid and gas phase in time while, on the other hand, the VoF method requires many computations and local refinements to identify the location of the thin interface between the two phases. Those problems can be solved by using a coupled method that applies both LS and VoF such that the combined modeling technique eliminates the drawbacks of each method and at the same time keep their advantages. In particular, with a combined method the user can have both track and control of the interface location with low computational cost.

There can be found many several coupled/ dual-interface methods in the literature. The slightly differences between the coupled methods are mentioned on the way of the interaction between LS and VoF method. The final choice for the combined solver for the interface simulation of the Taylor bubble flow depends on the user and at the problem's requirements for efficiency, accuracy and computational time. Some examples of dual-interface methods are the coupled volume-of-fluid and level set method (VOSET) [44], the adaptive coupled level-set/volume-of-fluid (ACLSVoF) method [45], the novel coupled method for unstructured meshes [46], the Mass-Conserving Level Set method (MCLS) method in Cartesian coordinates [47] and its' improvement in cylindrical coordinates [12]. At this literature study, the focus will be on MCLS method in cylindrical coordinates as this method may be the starting point of a future master thesis on high fidelity simulations of Taylor bubbles in co-current turbulent flow. The small differences between the methods can become comprehensible by studying the relevant literature.

The distinguishing feature of the Mass-Conserving Level Set method is that it achieves mass conservation by calculating the VoF value at each cell through the level-set function and its gradient. This feature can be applied both on a uniform Cartesian grid or a cylindrical grid and one of its' applications comprises the Taylor bubble flow. The MCLS method has been validated for indicating good levels of robustness and accuracy in comparison with the rest coupled methods [47], [12]. Moreover, the algorithm in cylindrical coordinates tried to eliminate all instabilities and possible singularities that may occur in the multiphase flow field, accomplish competent accuracy (minimum second order) and at the same time to be computationally cheap. The reason is that the algorithm is designed such that it can apply to turbulent flows where irregular fluctuations in time as well as in space, small as well as large three-dimensional eddies (vortices) coexist. To achieve this, the domain is limited to a straight, inclined, cylindrical pipe [12].

The MCLS algorithm is illustrated at figure 2.4. For clarity, the explanation of the algorithm will be done by keeping the same notation with the literature:

- The level-set or distance function of the center of each cell to the interface is given by $\phi_{i,k}^{(n)}$ at time step n.
- The volume fraction or volume value of the center of each cell at VoF is given by $\psi_{i,k}^{(n)}$ at time

step n.

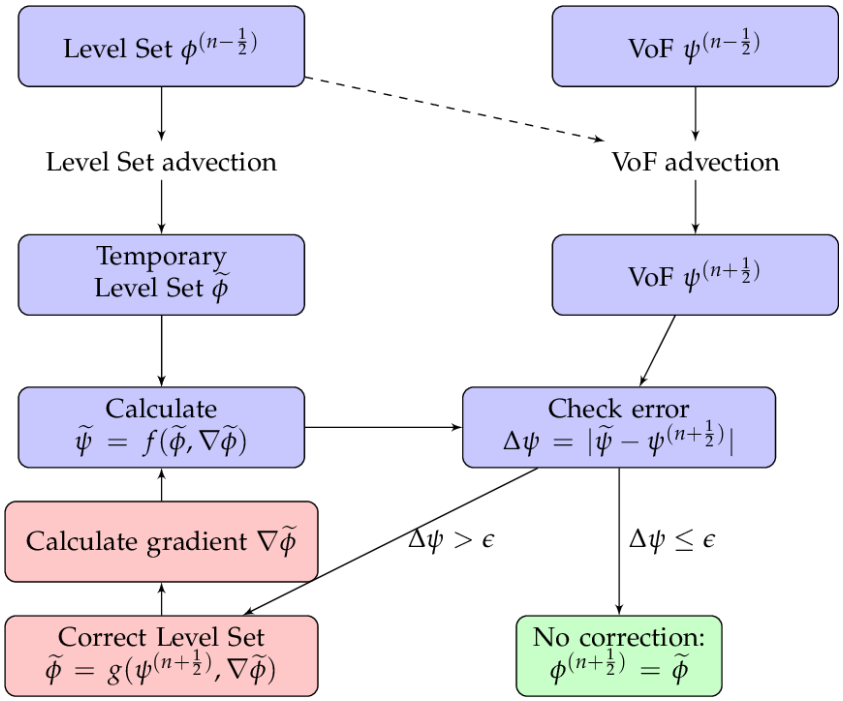

Figure 2.4: MCLS algorithm with Level-Set function ϕ, VoF function ψ: The left-hand side branch corresponds to pure Level-Set advection. The right-hand side branch represents the VoF advection [12].

The idea of the method is that we can fix the lack of the mass conservation LS method by applying some corrections to the Level-set function $\phi_{i,k}^{(n)}$ which are derived from volume fraction $\psi_{i,k}^{(n)}$ of VoF method for every cell and every time step. This is done with the following steps (2.4):

- Firstly, the LS function $\phi_{i,k}^{(n-\frac{1}{2})}$ and the VoF function $\psi_{i,k}^{(n-\frac{1}{2})}$ are advected together with the velocity field at the time step $n-\frac{1}{2}$.

- Then, by solving numerically the advection equation for LS, a first prediction of the level set $\tilde{\phi}_{i,k}^{(n+\frac{1}{2})}$ for each cell at the next time step is approximated. Simultaneously, the VoF fraction $\psi_{i,k}^{(n+\frac{1}{2})}$ is computed through its' advection algorithm for which it is known that the mass conservation property holds.

- Next, the computed accurate value of volume fraction $\psi_{i,k}^{(n+\frac{1}{2})}$ is compared at each mesh cell with an approximate value of volume fraction $\tilde{\psi}_{i,k}^{(n+\frac{1}{2})}$ obtained as the result of a non-linear function f which takes as arguments the approximate values $\tilde{\phi}_{i,k}^{(n+\frac{1}{2})}$ and $\nabla\tilde{\phi}_{i,k}^{(n+\frac{1}{2})}$ and maps them to the volume fraction of VoF. The comparison checks for each cell if the discrepancy between the approximated value and the accurate value of volume fraction of VoF method is smaller than a user-defined value ϵ. The choice of ϵ is important for the accuracy and the computational cost of the method.

- Depending on the result of the comparison, the initial approximation of $\tilde{\phi}_{i,k}^{(n+\frac{1}{2})}$ for every cell may (if discrepancy is bigger than ϵ) or may not be corrected (if discrepancy is smaller than ϵ).

- If a correction is need, the algorithm continues by computing a new approximated value $\tilde{\phi}_{i,k}^{(n+\frac{1}{2})}$ of level set function. This is done by calculating the inverse function of f, namely g, which takes

as arguments the computed accurate value of volume fraction $\psi_{i,k}^{(n+\frac{1}{2})}$ and the $\nabla\tilde{\phi}_{i,k}^{(n+\frac{1}{2})}$ from the initial guess.

- After calculating the new approximated value of level-set function $\tilde{\phi}_{i,k}^{(n+\frac{1}{2})}$, its' gradient is computed and a new approximation of $\tilde{\psi}_{i,k}^{(n+\frac{1}{2})}$ is obtained.
- The comparison check continues iteratively until the required tolerance is achieved for all cells. Then we can proceed with the next time step.

3

Software for the Simulation of Taylor Bubble Flow

There is a big variety of open source and commercial software packages that are widely used in research and industry for the simulation of the numerical models in the Taylor bubble flow. Since there is no analytical solution to the Navier-Stokes equations at Taylor bubble flow problem, the error of a simulation can be hard to quantify. This is the reason why an experiment is often chosen to confirm the findings of the simulations and the validation of theoretical models. Therefore, for the verification of the accuracy of CFD software in Taylor bubble flows, we intended to find articles where the results from simulation were also followed by experiments under the same physical flow conditions, e.g. same Reynolds number [5].

In cases where the simulation results are not followed by an experiment (due to cost or complexity of the flow), the researchers compare their findings with previous publications which simulated exactly the same problem under identical conditions but with different software or flow modeling method.

Last but not least, there are a few cases of papers with a code comparison for Taylor bubble flow simulations. Since each software package uses its own parameters and variables for describing the same problem, a mapping between the software's parameters was needed.

During the current literature study, an important parameter is the version of the software package that was used in the bibliography because the target was to capture the latest versions of each software. Therefore, the search was limited to the results from the last decade so that the most recent documents will be gathered.

3.1. Commercial software packages

VoF method has been known for several decades, has gone through a continuous process of improvement and is used by several commercially available software programs the last decades for simulation of rising bubble flow problems [48]. On the other hand, other numerical methods for multiphase flow modeling such as Level-set method, dual-interface methods, front-tracking methods, etc. have either recently or not yet been developed in the most popular packages [48]. Therefore, the only way to perform these methods is through user-defined functions such as in the recent numerical studies implemented in ANSYS Fluent [49], [50], [51], [52].

ANSYS Fluent is the most widespread CFD software package used for simulations of multiphase flows and in particular, for the motion of a rising bubble in a liquid. In ANSYS Fluent, there are both Eulerian-Eulerian two-fluid models and Lagrangian discrete phase models. For Taylor bubble flow, three different Euler-Euler multiphase flow modeling methods are available: the VoF, the mixture, and the Eulerian-Eulerian model [48], [53]. Front-tracking methods for flow modeling are not yet available on ANSYS Fluent and they can still be performed only via user-defined functions such as in [52].

The VoF model is the easiest and most popular method to be implemented in ANSYS Fluent, nevertheless, there are some limitations in the model's implementation and especially in the early versions [48]. For example, in Release 12.0 the restrictions in the use of VoF modeling contain that the

simulation can be implemented only by the pressure-based solver, stream-wise periodic flow cannot be used and second-order implicit time-discretization scheme is not possible [54].

Despite those restrictions, predictions from numerical simulations are found to be accurate even for early versions. For instance, the simulation of a Taylor bubble flow in both stagnant and flowing liquid is implemented in Fluent (Release 5.4.8) using VoF method in [23] and the findings are found to be in good agreement with experimental results obtained from literature [55].

However, in the early versions, the LS method is not available and therefore, a coupled LS and VoF method could be performed only via the tool of user-defined functions. For example, the coupled LS-VoF (CLSVoF) method for modeling of gas-liquid interface in bubbly flow as presented in [50]. The authors eliminated the drawbacks of both individual methods and achieved a CLSVoF method by using the available VoF method in ANSYS Fluent (version 6.3.26) and performing LS method via user-defined functions.

The latest versions of ANSYS Fluent show a significant improvement in the accuracy of the numerical simulations of Taylor bubble flow. For example, the VoF methodology of ANSYS Fluent (Release 12.0.1) is performed in the numerical survey about the rising of Taylor bubbles through a stagnant Newtonian liquid [56]. The results obtained for the velocity and the frontal radius of the nose of the Taylor bubble are favorably compared with a published collection of data from experimental measurements [57].

The next release (14.0) of ANSYS Fluent is the first version which had available the CLSVoF method so that the deficiencies of the LS method and the VoF method are overcome. The efficiency of CLSVoF method is illustrated in a numerical study for the bubble formation in a square microchannel with a converging shape mixing junction with background liquid flow [49]. The comparison between VoF and CLSVoF model of ANSYS Fluent indicated that with CLSVoF model a more accurate interface can be achieved especially at the rupture stage of the bubble and the bubbles obtained, were more consistent with the experimental outcome.

A finite-volume-based CFD solver ANSYS Fluent of Release 14.0 is also performed in the numerical simulation for the dynamics of bubble formation from two submerged orifices in an immiscible Newtonian liquid [58]. The dynamic effects of the quiescent and the co-flowing liquid ambiance on the bubble evolution and detachment processes were compared with experiments from literature [59].

Release 15.0 is applied for the simulation of rising Taylor bubbles in [20], [51]. In [20], VoF method is applied in the flow field and the values obtained are matching favorably with published experimental and other modeling findings [60] while in [51], a numerical study for the bubble dynamic behavior utilizing the coupled Level Set and Volume of Fluid (CLSVoF) method is illustrated. The authors in the latter study used also the tool of user-defined functions but only for the mass and energy transfer and not for the CLSVoF as in [50].

ANSYS Fluent 16.0 was used for performing a detailed numerical study focused on the mass transfer phenomenon from Taylor bubbles of pure oxygen to co-current liquid initially absent of solute is presented in [35]. The authors implemented a VoF method for capturing the interface accurately.

Another well-known commercial CFD software package is the STAR-CCM+ software. STAR-CCM+ offers a wide choice in modeling multiphase flows and is implemented in many researches flows such as in [61]. In this publication, the aim was to indicate the accuracy of numerical simulations using STAR-CCM+ (version 10.06.010) with VoF modeling in slug flow conditions and in particular, in Taylor bubble flow. STAR-CCM+ has been validated in several studies for Taylor bubble flow and can give accurate predictions. For example, in [61], the divergence of the prediction from experimental results is less than 2%.

Last but not least, NEPTUNE CFD, which is based on a finite volume approach, is a multiphase-flows solver which can be used for Taylor bubble flows like in [32]. NEPTUNE CFD is powered by Code Saturne HPC capabilities and can be embedded in the SALOME platform.

3.2. Open source software packages

Open-source means that the user is free to view and modify the underlying code of the software. This approach is beneficial to researchers in at least two ways; First, they can freely release their data and experiments so that anyone can replicate the study just by downloading and installing the software; Secondly, the original code is open to be read and so anyone can check the validity of either the mathematics or other technique's used in the publication. This can not always be done with commercial software packages, as not everyone has access to them because of their cost and the code, is often treated

as secret so no one can read it.

OpenFOAM is an open-source CFD software package and comprises a collection of C++ libraries. OpenFOAM and its' libraries are widely used for simulation of multiphase flows and in particular, Taylor bubble flows [62]. Until the last decade, OpenFOAM and most open-source CFD software packages were not yet released [63], and therefore, the majority of the CFD simulations in multiphase flows were done with commercial software packages. OpenFoam has a standard two-phase incompressible flow solver for VoF method, namely InterFOAM, which solves the two-phase equations of flow on collocated grids using finite volume discretization [13], [34].

A numerical prediction for the motion of Taylor bubbles rising in a liquid using OpenFOAM is presented in many studies. For example, OpenFOAM version 2.3 and its' multiphase solver InterFOAM is used in [34] while a modified version of the standard InterFOAM VoF solver (OpenFOAM 4.0) for unstructured grids is applied in [13]. The two main differences of the latter study from standard InterFOAM version are the lack of the dissipative term in the incomplete flux and the two-stage Diagonally Implicit Runge-Kutta (DIRK) for the time integration scheme. In both studies, the results are compared favorably with the other numerical and experimental results [64], [65], [66], [67], [56], [68].

Another efficient open-source code for Taylor bubble flows is the Parallel Hierarchic Adaptive Stabilized Transient Analysis (PHASTA). PHASTA software comprises a direct numerical simulation (DNS) flow solver which can model compressible or incompressible, laminar or turbulent, steady or unsteady flows in 3D, using unstructured grids. PHASTA adopts the LS and not the VoF method for the modeling of the interface of the two-phase bubble flow. PHASTA may give from second to fifth order of accuracy and is based on a stabilized formulation of Finite Element Method (FEM) and have been confirmed many times in the past for various configurations of bubble flows [69], [70]. For example, in [28], a three-dimensional numerical analysis of the dynamics of large deformable bubbles in pipes of different geometries and orientations was implemented using PHASTA. PHASTA is also used in a novel algorithm which has been recently published in order to prevent or delay bubble coalescence while simulating multiple bubble behavior using LS approach at large scale [26].

A parallel c++/ MPI code, called TermoFluids is designed for direct numerical simulation and large eddy simulation of turbulent flows and it is used in many studies. For example, a numerical study of Taylor bubbles rising in a stagnant liquid using a coupled conservative LS-moving mesh method is tested in [27]. TermoFluids was also used in the research for the simulation of single and multiple bubbles with the conservative LS method which is performed in [33]. The same authors use also TermoFluids in another two researches for multiphase flows; a coupled VoF/LS method for simulating incompressible two-phase flows on unstructured meshes and a finite-volume/level-set method for simulating two-phase flows on unstructured grids [46], [29].

Moreover, a novel numerical two-phase flow algorithm in cylindrical coordinates was implemented in FORTRAN 90 in [12]. The case of Taylor bubble flow in is tested and the accuracy of the code is compared with the results from other studies which used different software [19].

3.3. Comparison of CFD software

Regarding code comparison, some empirical parameters and model details have to be changed to obtain comparable agreement between different codes which simulate the same problem. Therefore, it is necessary to perform a mapping between the various software parameters to apply a comparison.

For example, a comparison of commercial software packages ANSYS Fluent and Transport phenomena Analysis Tool (TransAT) have been implemented for the simulation of bubbly flow case in [71]. VoF modeling is adopted in Fluent while LS model is selected in TransAT which is developed by ASCOMP GmbH [72]. The results indicate a recirculating flow for bubbles by TransAT while negligible recirculation was observed in the solution with Fluent. In general, the TransAT captured the instabilities and therefore, it predicted with better accuracy the slug flow in comparison with the experimental findings. The computation times between the two methods are similar.

A code comparison has been also implemented for dispersed bubble flow. For example, a code comparison between OpenFOAM (version 2.2.x) and ANSYS CFX for monodisperse bubbly flow was executed and their predictions are compared with results from experiments [73]. Another study for CFD simulations of a bubble column with and without internals compare results between OpenFOAM and ANSYS Fluent [74]. In both examples, comparable results obtained with both commercial and open-source codes (deviations around 3-4%) for different configurations of multiphase bubble flows in [74]

although some differences in the procedure remained [73]. For example, for the implementation of the turbulent wall functions in [73], cell-centered discretization is used in OpenFOAM while a vertex-based scheme is preferred in ANSYS-CFX. In general, although the experimental data are satisfactorily reproduced by the numerical simulations implemented in OpenFOAM, some deviations from experimental results have been identified.

Similar efforts for the comparison between open-source and commercial software packages and their matching with the experimental results have been also done for flows in micro-scale pipes (with a diameter of less than 1mm). An interesting research paper in this field was the numerical as well as the experimental examination of the dynamic behavior of isolated confined air bubbles in laminar fully-developed flows within circular channels of very small diameters [75]. The experimental results derived from the micro-particle velocimetry technique were compared with the outcome of the computational fluid dynamic simulations performed both in ANSYS Fluent v.14.5 and ESI OpenFOAM v.2.1.1. The paper concludes that numerical results coming from both ANSYS Fluent and OpenFOAM agreed well with the experimental results in the majority of cases (errors always smaller than 10%) and the discrepancies occurred between experimental and numerical bubble velocity and liquid film thickness are within the error bands of the experimental measurements. Only in cases of large capillary numbers, the results of the dynamics of the liquid film for air-water flows were slightly better using ANSYS Fluent in comparison with OpenFOAM because OpenFOAM resulted in narrower bubbles which led to errors in the surface tension forces. In the extreme case of significantly small capillary numbers, even the experimental results led to absolute errors up to 30% while in normal cases the error coming from experiments is assumed negligible or it is identified and subtracted [75].

4

Numerical Simulation of Taylor Bubble Flow

A large amount of studies is published every year in the dynamics of Taylor bubbles rising within vertical pipes which also contain viscous liquid. The reason is that the formation of Taylor bubble flow is met in many industrial applications such as in geothermal power plants, steam boilers, and heat exchangers in thermal power plants, oil extraction from wells, transportation of hydrocarbons through pipes, blood flows and in the emergency core cooling of nuclear reactors [21], [16], [13].

The shape of the Taylor bubble may be different even for the same application. In general, Taylor bubble is always bullet-shaped with a rounded leading edge, a cylindrical main part and either a more rounded or more flattened trailing edge. The width of the Taylor bubble usually conceives almost all cross-section of the pipe and therefore, a very thin film of liquid exists between the bubble and the pipe walls [13]. As this thin film decreases, a wake is created in the region behind the Taylor bubble. The wake region depends on the trailing edge of the Taylor bubble, fluid properties, flow conditions, and pipe geometry [16].

Taylor bubbles usually appear in sequences, i.e. behind a Taylor bubble another Taylor bubble is flowing with similar shape and velocity. The so-called liquid slugs which consist of smaller dispersed bubbles are present between two Taylor bubbles [16]. The distance between two Taylor bubbles also affects the wake region.

The behavior and motion of the Taylor bubble are affected by a group of non-dimensional numbers. The most important non-dimensional numbers for the Taylor bubble flow are the Eötvös (Eo) or Bond (Bo) number, the Morton (Mo) number and the Froude (Fr) number and are defined as:

- $Eo = \frac{\rho_l g D^2}{\sigma}$,
- $Mo = \frac{g\mu_l^4}{\rho_l \sigma^3}$,
- $Fr = \frac{U_t}{\sqrt{gD}}$,

where ρ_l is the liquid density, μ_l the liquid viscosity, g the gravitational acceleration, D the pipe diameter, σ the surface tension and U_t the terminal velocity of the bubble. In particular, Eo represents the ratio of capillary forces to gravitational forces and together with Mo number characterizes the shape of the bubble moving in a surrounding fluid while Fr is the ratio of the flow inertia to the external field (i.e. gravity). The Eo and Mo consists of the input parameters of a simulation while Fr is a number that comes from the outcome of the prediction [12].

However, to be able to sufficiently describe the Taylor bubble flow and derive the non-dimensional governing equations, it is necessary to define another few non-dimensional numbers: the Reynolds (Re) number (defined in general form in 1.3), the Archimedes (Ar) number, the Weber (We) as well as the density and viscosity ratio. These numbers are defined as:

- $Re = \frac{\rho_l U_t D}{\mu_l} = \frac{U_t D}{\nu_l}$,

- $Ar = \frac{\Delta\rho g L^3}{\rho_l \nu_l^2}$,
- $We = \frac{\rho_l U_t^2 D}{\sigma}$
- $\lambda = \frac{\mu_l}{\mu_g}$,
- $\eta = \frac{\rho_l}{\rho_g}$,

where $\Delta\rho = \rho_l - \rho_g$ is the density difference and ν_l the kinematic viscosity of the liquid. The Re depicts the ratio of inertia to viscous forces, the Ar the ratio of gravitational forces to viscous forces while Weber number represents the fluid's inertia compared to its surface tension.

The problem becomes more complex as the liquid flow is increasing from stagnant to laminar and then to turbulent flow [21]. In this chapter, predictions of numerical simulations in Taylor bubble flow which was found in the literature are presented together with their achieved accuracy compared to experimental findings or results from other publications. Taylor bubble flow problems are very complex problems due to the aperiodic and unsteady behavior both in space and time and therefore, there are some restrictions at studies coming only from experimental work without using any simulation [16], [66].

All numerical simulations of rising Taylor bubbles in pipes through liquid background flow are taking into consideration some assumptions in order to reduce the complexity, and therefore the computational cost, of the problem. For example, the majority of numerical simulations of rising Taylor bubbles in pipes with laminar or stagnant liquid background flow are simplified into two dimensions. The reason is that the liquid flow along the Taylor bubble is laminar and axisymmetric, and therefore, its motion is governed by a two-dimensional momentum equation which less complex. Moreover, in simulations of stagnant liquids with high viscosity, the predictions lead to steady behavior of Taylor bubbles. However, this assumption leads to some numerical errors and they cannot capture the realistic flow.

As a consequence, the complexity of the dynamics of the Taylor bubble depends on the background liquid flow. Therefore, the current research is divided into three main subsections depending on the background liquid flow within the vertical tube. In particular, the studies are divided into stagnant, laminar and turbulent background liquid flow. In most of the literature, the analysis is done on co-current flow of the rising Taylor bubble, which means that the Taylor bubble flows in the same direction as the buoyancy force. For example, a schematic sketch of a (half) Taylor bubble rising within a tube filled in with co-current liquid is illustrated in figure 4.1 as presented in [21].

4.1. Stagnant liquid

The pioneer research on rising Taylor bubbles was carried out in [76] and [77]. Since there was neither simulation tools nor experimental findings, it was only theoretically found that the rising velocity of a Taylor bubble in an inviscid flow was $U_o = \alpha\sqrt{gD}$ where α is a coefficient with value between 0.33 and 0.35. The results of the above studies have been validated experimentally later in [78], [79].

A stabilized finite element method with LS modeling of the interface for the three-dimensional computation of incompressible bubble dynamics within a quiescent liquid is illustrated in [70]. The results from the three dimensional analysis indicate that the capability of the method to manage the bubble coalescence and breakup.

Numerical simulations for three different cases of laminar Taylor bubble flow in a stagnant liquid have been implemented in [13], amongst others. The three cases which were tested are convex tail without wake, concave tail without wake, and concave tail with wake. A Moving Frame of Reference (MFR) is attached to the Taylor bubble and non-periodic inlet and outlet boundary conditions are used. The predictions coming from the modified InterFOAM compare favorably with the experimental results from [66], [67] and the numerical models of [56]. The small deviations are justified by some unsteady behavior near the tail of the Taylor bubble.

A numerical study of Taylor bubbles rising in a stagnant liquid is illustrated in [27]. The governing equations have been discretized on a collocated unstructured grid arrangement with a central difference scheme of the Finite Volume Method (FVM), according to [29] in which rising gas bubbles are simulated in quiescent liquid on unstructured grids. Both studies used TermoFluids for their simulations. The results of the former study show very small deviations from experimental findings [24] and other numerical studies [80], and therefore, the numerical prediction is characterized as accurate.

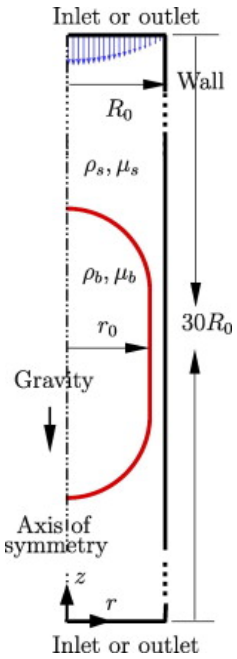

Figure 4.1: Schematic sketch of a (half) Taylor bubble rising in a cylindrical tube filled with co-current liquid as shown in [21]. The co-current liquid can flow upwards or downwards. The Taylor bubble flow within a pipe is an-axis symmetric problem and it is usual to do the half sketch.

A conservative level-set (CLS) method has been used to study the buoyancy-driven motion of single and multiple bubbles on a one-directional periodic domain through a stagnant liquid in [33]. The equations of CLS have been discretized on a collocated unstructured mesh with a Finite Volume Method and a central difference (CD) scheme is used to discretize the convective term. The simulations were implemented in Termofluids and the predictions are found to be in good agreement with experimental and numerical results from the literature such as in [81] and [82].

Rising Taylor bubbles through stagnant liquid is also performed in the simulation in [50]. At this study, a fully three dimensional Cartesian level set method was coupled with the volume of fluid method within ANSYS Fluent version 6.3.26 which uses a staggered Finite Volume code. The level set was discretized with a fifth-order weighted essentially non-oscillatory (WENO) scheme for spatial derivatives and a first-order Euler explicit method for temporal discretization. The method was implemented on both serial and parallel solvers. In the end, they compared the CLSVoF method with the original VoF and conclude that CLSVoF acquires better accuracy. In particular, the deviation from experiments was less than 16% using CLSVoF whereas with VoF the maximum relative error was approximately 19%.

A three-dimensional simulation has been also applied for Taylor bubble turbulent flow in initially stagnant liquid in [61]. The experiment published in [83] is used as a reference for all calculations. LES calculations implemented with STAR-CCM+ give less than 2% error for a well-refined mesh. The dependency of the results from mesh size and Courant number were assessed in this work.

A complete dimensionless analysis of single Taylor bubble rising through a vertical stagnant Newtonian liquid problem is carried out in [20]. The FVM is used to discretize the governing equations. Using VoF method in ANSYS Fluent, good approximations are found for Taylor bubble's shape and velocity, flow in the liquid film region and flow in the wake region with respect to the experiments [66] and other theoretical models [57].

Stationary liquid is also used in the numerical simulation of Taylor bubbles rising in a vertical tube at [22]. A Finite Difference Method is used for the discretization of NS and VoF for capturing the gas-liquid interface. The simulation was executed with ANSYS Fluent and was matching well with the experimental findings in the literature [84].

Last but not least, similar simulations have been carried out in [34] where Taylor bubbles with turbulent wake and their coalescence have been investigated. An OpenFOAM solver using VoF modeling and FDM discretization gave accurate predictions for void fraction, mean Taylor bubble velocity and turbulent fluctuations. The results were compared favorably with experimental findings [64].

4.2. Laminar liquid flow

In several studies, the motion of Taylor bubbles in vertical tubes through both stagnant and laminar flowing liquids are illustrated and therefore, it is difficult to categorize them. Examples of this case are indicated in [23] and in [46] where a novel coupled method for unstructured meshes is presented. Initially, the liquid is quiescent, but as the Taylor bubble is moving up, the liquid ahead of the bubble is starting to accelerate downwards until it reaches a maximum terminal velocity. The distance between the front nose of the Taylor bubble and the accelerated liquid is smaller for slower bubbles. The same time at region at the rear of the bubble, a wake may appear which depends on the inverse viscosity dimensionless number N_f. The results of the simulation in [23], which was performed with Ansys Fluent using the VoF method, agree fairly well with experimental and numerical results from the literature. In particular, the shape and velocity of the slug, the velocity distribution and the distribution of local wall shear stress illustrate a great matching with [84].

Numerical predictions for Taylor bubble flow in both co-current and counter-current flow with laminar background liquid flow are presented in [21]. The front tracking method for interface capturing together with the finite difference method for Navier-Stokes equations are used for the dynamic analysis. The Crank Nicholson method is applied for the time integration. The results show that when the co-current flows in the same direction with the buoyancy (i.e. upward flow), the bubble is elongated and the flow separation at the elongated tail is easier. On the contrary, when the co-current flows on a rising Taylor bubble in the direction opposite to the buoyancy force (i.e. downward flow), the bubble becomes fatter and shorter, the tail's shape is more rounded for large Ar numbers and therefore, the flow separation is more difficult.

A new dual-interface capturing method for axisymmetric flows is presented and it is tested for the Taylor bubble case in [12], amongst others. The spatial discretization of the Navier-Stokes equations is implemented by using a second-order accurate finite difference approach as presented in [85]. The momentum equations are linearized with Newton linearization, and the discretization in time is done with an Implicit Midpoint time integration method. The Poisson equation for the pressure is solved by implementing the Conjugate Gradient (CG) method. The simulation is implemented in FORTRAN for two low-viscosity cases and three moderate-viscosity cases and the results are compared with the numerical results of [19] as well as the experiments of [84] and [24]. The deviation of the output Fr number is found to be around 1% in comparison with the numerical simulations of [19]. In general, for all cases, the shape, and the terminal velocity are in agreement with the numerical and experimental findings from literature except for one case of large Reynolds numbers where the bubble breaks up after some time.

A three-dimensional numerical analysis of the dynamics of large deformable bubbles in pipes of different geometries and orientations for laminar liquid flow was investigated in [28]. The reference for the formulation of the three-dimensional set up of the bubbly flow is the experimental conditions used in the literature [86]. Due to the axis-symmetry and the laminar flow, the problem is described by the governing equations in two dimensions. The results derived from numerical predictions are found to accurately matching with those from both experiments and theoretical models for all configurations.

Simulation of rising Taylor bubbles for varying inlet liquid velocities but always within the laminar range is executed in [35]. For achieving constant solute concentration at the bubble surface, the flow domain is solved by coupling the VoF method with a geometric reconstruction scheme which uses PLIC method as applied in [39]. The simultaneous solution of the flow field, bubble shape, and mass transfer in a domain with stationary walls was predicted accurately. However, the results obtained by ANSYS Fluent for the mass transfer coefficient data from soluble bubbles showed a remarkable divergence in comparison with the existing theoretical models [87], [60]. The reason for this difference can be explained by implementing the relevant experiments.

Two different codes, Transat and ANSYS Fluent, were compared each other for the accuracy of their predictions for the case of rising bubbles in laminar co-current liquid flow, amongst others [71]. The codes use different spatial and space discretization schemes as well as interface tracking methods. The simulation in Transat was executed with LS interface capturing method, 3rd order Quadratic Upstream Interpolation for Convective Kinematics (QUICK) for spatial discretization and 3rd order Runge-Kutta for time discretization. On the other hand, ANSYS Fluent uses a VoF method, 3rd order Monotonic Upwind Scheme for Conservation Laws (MUSCL) and 1st order Euler correspondingly. Computational times, complexity, accuracy, consistency, recirculation, and stability are checked for both codes and the results are compared with their deviation from experiments found in the literature [88].

4.3. Turbulent liquid flow

A Large Eddie Simulation (LES) of turbulent co-current Taylor bubble flow is illustrated in [13]. According to the knowledge of the author, this is the only publication that can be found in the literature which presents a fully three-dimensional simulation that can reproduce the motion of an individual Taylor bubble in a turbulent co-current background liquid flow. After the validation of the predictions of laminar Taylor bubble flow in a stagnant liquid, a simulation is performed for a turbulent co-current Taylor bubble flow. For the discretization in space, the finite volume method has been used but for the computation of the interpolated velocity at the face of each control volume near the free surface, the authors used a blended scheme to verify stability. In particular, at the free surface, a Van Leer scheme is used which stabilizes the free surface and suppresses artificial bubble formation together with a second-order central difference scheme. A second-order accurate diagonally implicit Runge-Kutta scheme is used for the temporal discretization. The accuracy of the numerical simulation is compared with the findings of [65] for single-phase turbulent pipe flow while for the final case which comprised the three-dimensional simulation of a Taylor bubble in a turbulent liquid flow and was compared with experimental measurements from [68]. For all cases, the prediction models agree with the published data from the literature except for an underestimation of the fluctuating velocities close to the Taylor bubble due to the laminarization of the flow in the wake region.

5 Conclusion

This literature study provides the theoretical background necessary for understanding the problem of Taylor bubble flow rising in pipes with a liquid background flow and provides most of the up-to-date relevant research that has been published. The motivation for this work comprises both the wide variety of engineering systems in which the Taylor bubble flow is encountered as well as the scientific gap that was found. The three main interface modeling methods have been explained in detail and the capabilities and restrictions of each software that has been used in similar studies are indicated. After analytical research, the lack of realistic and accurate data in the laminar, transitional and turbulent co-current flow has been identified and the future master thesis will try to fill a part of this scientific gap.

In particular, this literature study prospects on performing a high fidelity simulation of Taylor bubbles in co-current turbulent flow. The simulation will be performed in cooperation with the research and innovation unit of NRG. Corresponding research questions, goals and approach are stated in this chapter prospecting on the remaining part of the master thesis.

5.1. Discussion

Numerical simulations of rising Taylor bubbles in pipes through liquid background flow are complex and unsteady problems. Most of the studies found in the literature and presented in chapter 4 try to decrease the complexity and the computational cost. For example, reduction of mesh size and use of symmetry of the flow problem were widely used in most of the studies.

Table 5.1 summarizes the main sources that are found in the literature for the numerical simulation of rising Taylor bubbles within pipes through a background liquid flow. The first column indicates the source, the second the interface tracking method, the third the spatial discretization method, the fourth the software package used for the simulation and the last one depicts the type of background liquid flow. It can be observed that almost all studies which implement simulations of Taylor bubbles in stagnant or laminar liquid background flow while only [13] simulates Taylor bubbles in co-current turbulent flow .

According to the research of [16], despite the amount of studies performed, there is a lack of realistic accurate data in the case of not only turbulent but also transient or even laminar liquid co-current flow. The reason is that important assumptions and different constraints which are used in order to reduce the degrees of freedom, like symmetry or choice of a coarse grid, may affect the consistency of the results. In simulations of stagnant liquids with high viscosity, the predictions lead to steady behavior of Taylor bubbles. Even in simulations where the liquid flow along the Taylor bubble is laminar and axisymmetric, its motion is governed by a two-dimensional momentum equation which is simpler but gives less accurate and less realistic results [61], [23]. The same opinion is illustrated by the authors in [28]. In this study, it is also mentioned that it is necessary that the predictions of numerical simulations should not only be compared against specific experimental results but also to be carefully checked for their physical consistency and restrictions.

However, in many engineering problems of rising Taylor bubbles, the liquid background flow is turbulent and unsteady vortices of different sizes are created which interact with each other and increase

Table 5.1: This table displays the interface modeling techniques, the spatial discretization method, the software and the type of background liquid flow used for each numerical simulation of Taylor bubble flow found in the literature.

Author-source	interface modeling	spatial discretization	software	liquid flow type
Oud, [12]	MCLS	FDM	FORTRAN	laminar
Frederix, [13]	VoF	FVM	OpenFOAM	turbulent/ stagnant
Montoya, [61]	VoF	FVM	STAR-CCM+	stagnant
Taha, [23]	VoF	FVM	ANSYS Fluent	stagnant/ laminar
Massoud, [20]	VoF	FVM	ANSYS Fluent	stagnant
Quan, [21]	FT	FDM	not mentioned	laminar
Bugg, [22]	VoF	FDM	ANSYS Fluent	stagnant
Talley, [26]	LS	FEM	PHASTA	stagnant
Gutiérrez, [27]	CLS	FVM	TermoFluids	stagnant
Behafarid, [28]	LS	FEM	PHASTA	laminar
Balcázar, [29]	LS	FVM	TermoFluids	stagnant
Sussman,[30]	LS	FDM	not mentioned	stagnant
Mimouni, [32]	LS	FVM	NEPTUNE CFD	laminar/stagnant
Balcázar, [33]	CLS	FVM	TermoFluids	stagnant
Shaban, [34]	VoF	FDM	OpenFOAM	stagnant
Silva, [35]	VoF	FEM	ANSYS Fluent	laminar
Balcázar, [46]	CLSVoF	FVM	TermoFluids	stagnant
Dang, [49]	CLSVoF / VoF	FVM	ANSYS Fluent	laminar
Nichita, [50]	CLSVoF	FVM	ANSYS Fluent	stagnant
Igaadi, [51]	CLSVoF	FDM	ANSYS Fluent	stagnant
Hua, [52]	FT	FVM	ANSYS Fluent	stagnant
Araújo, [56]	VoF	FVM	ANSYS Fluent	stagnant
Prasad, [58]	VoF	FVM	ANSYS Fluent	stagnant
Nagrath, [70]	LS	FEM	not mentioned	stagnant
Carlson, [71]	LS / VoF	QUICK/MUSCL	TransAT/ANSYS Fluent	laminar

the complexity of the problem due to their chaotic behavior. Therefore, an accurate prediction requires a fully three-dimensional analysis. For example, in the design and operation of a nuclear facility, it is important to understand the behavior of Taylor bubble flow in all flow regimes and all types of liquid background flow, including turbulent. The scientific gap of the simulations of Taylor bubbles in co-current turbulent flow is a challenging topic and comprises the ambitious target of the upcoming master thesis which will be carried out in collaboration with NRG.

5.2. Preliminary Research Questions

Each of the different multiphase flow regimes can be a thesis project in itself, therefore during the upcoming master thesis work the main focus will be how to successfully tackle high fidelity simulations of Taylor bubbles in co-current turbulent flow, using the Basilisk code. To achieve reliable predictions, the following approach will be followed:

- Learning Basilisk. Basilisk is an open-source flow solver that employs the Volume of Fluid approach for the modeling of two-phase flow [89]. One of the main features of Basilisk is the fact that it can perform local grid refinement.
- Identification and development of several simple test cases, for example in the dam break problem or in rising bubble cases, to be simulated with Basilisk and to be post-processed.
- Validation of the Basilisk solver in the setting of single-phase turbulent channel and pipe flow.
- Simulation of laminar Taylor bubble flow based on [56].
- Development of a high-fidelity simulation of Taylor bubble in co-current turbulent flow and comparison against either experimental findings from literature such as in [68], [90], [91] or NRGs OpenFOAM simulation results [13].

In the numerical analysis of Taylor bubbles in co-current turbulent flow using Basilisk, there are some critical issues that have to be taken into account and several corresponding sub-questions to be answered:

- By default the domain on which the equations are solved in Basilisk is a square box (or cube in 3D). How can the domain of pipe flow problem be constructed? How can we simulate a fixed wall?
- The problem is transient due to strong shear stresses, which leads to a continuous and progressive reduction in Taylor bubble's size (i.e. at the tail). What averaging strategy and what mesh size will be used?
- The small bubbles which are expected to break up from the Taylor bubble may either merge again with the Taylor bubble or may be transported downstream of the flow. Is this break up physical and how can it be verified that our results will be realistic after the break up?
- Which spatial discretization scheme for the divergence terms will be used to avoid instabilities of the free surface?
- Due to wall friction, the liquid flow loses kinetic energy and it is driven by a constant and spatially uniform pressure gradient. Therefore, even for high Reynolds number, laminarization of the liquid flow can be observed due to the thin liquid film between the Taylor bubble and the wall [92]. How can we keep the liquid flow turbulent?

Taking the above into consideration, we come up to the main research question:
What simulation strategy can be developed in Basilisk to accurately reproduce the motion of an individual Taylor bubble in both laminar and turbulent co-current background liquid flow?

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