RANS modeling of Taylor bubble flow
Relevant to nuclear reactor safety scenarios

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Relevant to nuclear reactor safety scenarios

Master of Science Thesis

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Ahmed Shekib Hamraz

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Preface

This document is the final report for obtaining the degree of Master of Science in Aerospace Engineering (AE) at Delft University of Technology (TU Delft). The thesis project is carried out at Research and Innovation department of Nuclear Research and Consultancy Group (NRG) in Petten, The Netherlands, and at department of Aerodynamics of AE TU Delft.

I would like to express my sincerest gratitude to Dr. ir. Marc Gerritsma, my university supervisor, Ed Komen, my supervisor at NRG, and Dr. ir. Edo Frederix, my daily supervisor at NRG, for their continuous support and guidance during this project. Multiphase flows was entirely new for me, Ed’s and Edo’s input was pivotal. Our discussions have every time motivated me and guide me to the right direction. The collaboration made my masters thesis project not only both challenging and interesting, but also lead to a paper that is currently being submitted. I am very grateful to Dr. ir. Afaque Shams and Ed Komen who gave me the opportunity to do my thesis at NRG. I would like also to thank Dr. Arne Siccama for his expertise for generating the meshes. Last but not least, I feel grateful for the unconditional love and support of my family and friends throughout my studies, it wouldn’t have been possible without them.

Delft, The Netherlands

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Abstract

In Pressurized Thermal Shock (PTS) applications, there is a co-existence of different flow regimes. The regimes can be divided in two main groups namely, dispersed two-phase flows and the separated two-phase flows having relatively larger interface. Simulating a two-phase flow itself is already a complex task. It gets even more complex when the flow is turbulent. Each phase can be laminar or turbulent depending which one is taken as point of reference. Primary phase may be turbulent compared to secondary phase but may be laminar compared to the vessel.

The objective of this master’s thesis project is Computational Fluid Dynamics (CFD) modeling of two-phase stratified flow settings relevant to Nuclear Reactor Safety (NRS) scenarios more specifically, the focus is placed on the modeling of Taylor bubble co-current flow (air-water) in a vertical pipe in Two-Dimensional (2D) and Three-Dimensional (3D). This is done through the application and validation of i) OpenFOAM’s standard VOF solver in combination with a conventional RANS model to mimic the turbulence behavior of the flow, and ii) NRG’s Runge-Kutta (RK) VOF solver in combination with a modified RANS model to capture the turbulent two-phase flow with large interfaces. For the purpose of this project two data sets are selected against which the morphology of the Taylor bubble is compared, namely the analytical model of Tomiyama et al. [1] and the high resolution Taylor bubble LES data of Frederix et al. [2].

It is shown that in case of i), where standard $k-\varepsilon$ is applied to model the turbulence behavior, the model fails to predict the interface of entire Taylor bubble adequately. This is because standard RANS models, which are initially developed for single-phase flows, overpredict the turbulence intensity near the interface. This is due to excessive turbulence production. This problem is addressed a.o. by Egorov et al. [3] who developed a model with a turbulence damping term in the turbulence model. This term is activated locally at the interface. Frederix et al. [4] have extended the Egorov approach in order to make it even more stable and robust. Frederix’s model is applied in ii) where it is shown that for a damping term, length scale, $\delta/D = 3.9 \times 10^{-3}$ the turbulence model is damped at the interface while in the rest of the flow the turbulence behavior is modeled properly by $k-\omega$ SST model.
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Chapter 1

Introduction

This report presents the thesis work that focuses on Computational Fluid Dynamics (CFD) modeling of a multiphase flow regime relevant to Nuclear Reactor Safety (NRS) applications. More specifically, the two-phase Pressurized Thermal Shock (PTS), which is related to Pressurized Water Reactor (PWR)- Reactor Pressure Vessel (RPV) lifetime safety studies. In PTS applications, there is a co-existence of different flow regimes. The regimes can be divided into two main groups namely, the dispersed two-phase flows (e.g. bubbly flows) and the separated two-phase flows having relatively larger interface (e.g. stratified flows, Taylor bubble flows, annular flows etc). This is explained adequately by Strubelj et al. [13] and Lucas et al. [14, 15].

The project is conducted at Research & Innovation department of Nuclear Research & Consultancy Group (NRG) at site Petten, Netherlands. NRG is specialized in developing and providing of sustainable nuclear technology for energy, environment, and health care. The company offers a wide range of services to energy utilities, government organizations and various branches of industry - including the nuclear, financial services and medical sectors. Furthermore, NRG is a major producer of medical isotopes in Europe. Besides the nuclear reactor applications the context of this report is also relevant for any other engineering application related to two-phase turbulent vertical pipe flows. Since the current is related to the nuclear reactor application, the next section introduces the nuclear reactor.

Furthermore, since the project is related to PTS applications Section 1.1 introduces the nuclear reactor shortly. This is will be followed by Section 1.2 where the objective of this report will be pointed out. The chapter closes with Section 1.3, where the outline of this report will be presented.
1.1 Nuclear reactor

A nuclear reactor is the main device of nuclear power plant, nuclear research facilities or a nuclear powered space vehicles, submarines and naval ships. It produces and controls the release of energy from splitting the atoms of certain elements. The evolution of nuclear reactors can be categorized in four generations. The generation I reactors are the prototypes and power producing non-commercial research reactors. The generation II were first commercial reactors that were built to be profitable and reliable. These reactors were operational from late 1960s. The generation III reactors are essentially extended from generation II reactors with evolutionary design improvements. The goal of these improvements were to expected the operational life of the reactors longer. The generation IV reactors are under development and the first commercial reactors of this kind is expected to be built in 2030s. Accordingly, each generation is classified by the type coolant. The most popular Reactor Pressure Vessels (RPVs) are the water cooled reactors that are divided in three categories, namely Pressurized Water Reactors (PWR), Boiling Water Reactors (BWR) and Pressurized Heavy Water Reactors (PHWR).

The integrity of the RPV is one of the main safety concerns at nuclear power plants. Within the reactor safety Pressurized Thermal Shock (PTS) plays a central role. PTS refers to a circumstance that threatens the integrity of the RPV. For a PTS analysis a multi-disciplinary approach is needed in order to include a wide range of issues that must be considered. Three conditions are typically essential that lead to a PTS safety concern:

1. neutron embrittlement of the RPV,
2. if the vessel has a pre-existing flaw of a critical size this will propagate rapidly through the brittle vessel, and
3. resulting to a rapid drop in temperature in the system (i.e. thermal shock).

This sequence of process is known as PTS. A severe PTS scenario takes place when cold water Emergency Core Cooling (ECC) is injected into the cold leg. The cold water mixes with the hot fluid already present in the cold leg. In such a PTS event different turbulent two-phase flow regimes are in co-existence or in transitional form present.

A full scale experimental test that could mimic the whole ECC injection process considering the various two-phase flow regimes are not feasible. Therefore, reliable numerical simulations are required. Computational Fluid Dynamics modeling of a turbulent two-phase flow regimes is a challenging task. The ongoing research has already performed simulations of isolated flow regimes with moderated success. It is reported that the treatment of the liquid/gas interfaces and the turbulences modeling, of both the liquid and the gas phases, and the coupling of these two turbulence fields, are most critical and difficult. On the other hand, the lack of accurate experimental data against which one could validate the model. Furthermore, in case if there are several two-phase flow regimes that co-exist, different models have to be applied for the same phenomenon. Furthermore, the modeling multiphase flows get even more complex.
when the flow is turbulent. Each phase can be laminar or turbulent depending from point of reference. Primary phase may be turbulent compared to secondary phase but may be laminar compared to the vessel. Other challenges are for example is density change across the phase interface is large $\rho_{\text{WATER}} \approx O(10^3)$.

### 1.2 Research objectives

The objective of this master's thesis project is CFD modeling of two-phase stratified flow settings relevant to Nuclear Reactor Safety (NRS) scenarios more specifically, the focus is placed on the modeling of Taylor bubble flow (air-water) in a vertical pipe in Two-Dimensional (2D) and Three-Dimensional (3D). This is done through the application and validation of

1. OpenFOAM’s standard VOF solver in combination with a conventional RANS model to mimic the turbulence behavior of the flow, and
2. NRG’s Runge-Kutta (RK) VOF solver in combination with a modified RANS model to capture the turbulent flow

For the purpose of this project two data sets are selected against which the morphology of the Taylor bubble is compared. Accordingly, the project is divided in two parts. The first part of the project comprises validation of Taylor bubble simulation by comparing the morphology of the bubble against the analytical model of Tomiyama et al. [1]. In the second part of the project the morphology of the bubble is compared against high resolution Taylor bubble LES data of Frederix et al. [2]. For the modeling of turbulence behavior, in part 1 use is made of a conventional RANS model while in part 2 modified RANS model is applied which is developed for two-phase flow with large interfaces, such as a Taylor bubble. The implementation and simulation strategy of part 1 and 2 are broken down in the following sub-goals, respectively.

- **Part 1: Validation against an analytical model of the standard VOF solver:**
  1. Selection of an appropriate dataset from Tomiyama et al. [1] which reflects the Taylor bubble regime, and an inventory of the flow conditions, required simulation geometry, initial conditions and boundary conditions.
  2. Generation of two-dimensional meshes (a wedge): a coarse, medium and fine mesh.
  3. Selection of the appropriate boundary conditions, based on simulation results.
  4. Grid convergence study.
  5. Bubble shape sensitivity analysis.
  6. Three-dimensional simulations of the complete setting using the optimal boundary condition strategy, and comparison against Tomiyama et al. [1].

- **Part 2: Validation against high resolution LES data of the RK VOF solver:**
  1. Selection of three-dimensional meshes, i.e., a coarse, medium and fine mesh.
2. Selection of an appropriate RANS turbulence model.
3. Implementing NRG’s modified RANS turbulence model.
4. Simulation of Taylor bubble formation in the same setting as NRG’s LES data set for the chosen flow conditions on three-dimensional meshes (i.e., a coarse, medium and fine mesh), and comparison against the LES data.

At the end of this report the following questions should be answered:

- is OpenFOAM’s standard VOF solver with a conventional RANS model able to model turbulent Taylor bubble flow?
- is NRG’s Runge-Kutta (RK) VOF solver with the modified RANS able to model turbulent Taylor bubble flow?

1.3 Thesis report organization

The outline of this report is as follows. Chapter 2 presents the background information by summarizing main state-of-the-art literature review, addressing the numerical methodology and describing the CFD solver. The results and the corresponding numerical models and methods, i.e. meshes, turbulence model etc., are divided in three chapters. Chapter 3 discusses 2D morphology validation of Taylor bubble against an analytical model using the standard VOF solver with \( k-\varepsilon \) model. This is followed by Chapter 4 where the bubble shape sensitivity is tested due to three parameters. In Chapter 5 the 3D Taylor bubble morphology validation is performed against high resolution LES data while use is made of RK VOF solver with the modified \( k-\omega \) SST model. Afterwards, Chapter 6 gives a summary and concluding remarks of this report. Finally, the recommendations for further work are given in Chapter 7.

But as already mentioned, the next chapter presents the relevant background information.
Chapter 2

Background

The contents of this chapter are meant to present background information relevant to this project. Accordingly, through a literature review the state of the art of this subject is shown. Beside, a compact review about the numerical methodology is presented, that can been seen as a short summary of several published works. The organization of this chapter is as follows. In Section 2.1 the multiphase flows are introduced. That is followed by Section 2.2 where the numerical methodology is presented. Modeling of slug flows is addressed in Section 2.3. The CFD toolbox in which simulation are performed is introduced in Section 2.4.

2.1 Multiphase Flows

A multiphase flow is a fluid flow consisting of more than one state or phase (i.e. gas, liquid or solid) and or different chemical properties in the same state or phase (i.e. liquid-liquid systems such as oil-water). Multiphase flows should have some level of phase separation at a scale well above molecular level. When a flow has a mixing on the molecular level, as such that there is no clear separation at macroscopic level by means of an interface, then it is known as multisppecies flows. The importance of multiphase flow has always existed both in natural phenomena and in industry application. Some of the industrial applications are power systems, heat transfers systems, process systems, transport systems, lubrication systems, biological systems. Some of the natural phenomena where multiphase flows plays a role are river flooding, ocean waves, formation and motion of rain droplets and of clouds. The dynamical behavior of all these applications and phenomena are described by the same physical laws, namely transport of mass, momentum and energy. In the past the design methods concerning multiphase flows were exclusively based on static-experimental correlations. With rapid advance in computational capabilities, the demand for progressively more accurate predictions for safe and economically sound operations are increased. Hence, to cope with these demand, mathematical models that can predict dynamical behaviors of multiphase flows are needed. It should be clear that the importance of multiphase flow is unmissable in the existing engineer-
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ing technology and with better understanding and prediction of it the importance will only increase. Multiphase flows exists in different forms, a common class of it is two-phase flows. In the current project the focus lies on two-phase flows. Two-phase flows consists of one or more interface and discontinuities at the interface. An interface refers to a finite thickness layer between two phase where material properties change. It is handy to classify two-phase mixtures according to the state of the different phases as follow:

- gas-solid mixture
- gas-liquid mixture
- liquid-solid mixture
- immiscible liquid-liquid

The gas-liquid mixture is based on the interface structures, which continuously changes. Therefore, the topological distribution of each phase is very difficult to compare with other mixtures. The class gas-liquid mixture, more specifically air-water is taken as primer class of two-phase flows throughout this report.

This section is dedicated to fundamentals of multiphase flows. In Subsections 2.1.1, the flow regimes that are present in a multiphase flow are presented. Subsection 2.1.2 deals with basic parameters and dimensionless numbers.

2.1.1 Flow regimes

Two-phase flows are categorized according to the morphology of the interfaces. The two phase flows are classified and some of typical flow regimes are listed as follows.

- separated flows consisting of:
  - stratified flows (free surface flows): immiscible fluids separated by a clearly-defined interface
  - annular flows: continuous liquid film with gas in the core and vice versa
  - jet flow: gas jet in liquid and vice versa

- transitional or mixed flows consisting of:
  - slug (churn) turbulent flow: large gas pockets in the continuous liquid

- dispersed flows consisting of:
  - bubbly flow: gas bubbles in a continuous liquid
  - droplet flow: liquid droplets in continuous gas
2.1 Multiphase Flows

Some of these flow regimes are illustrated in Figure 2.1, which is adapted from Weisman [5]. These sketches show the flow regimes in a vertical pipe for bubbly, slug, churn, annular and disperse flows, respectively. Figure 2.2 shows the images taken during experiments of two-phase (air-water) flows, adapted from Ishii et al. [6]. The experiments are performed in a vertical pipe with a diameter of 25.4 [mm]. From left to right the images represents, bubbly, cap-bubbly, slug, churn, and annular flow, respectively. In addition to the sketches and images from Figures 2.1 and 2.2, another useful tool to distinguish the various two-phase flow regimes are the so called flow regime maps. There are two kind of flow maps namely, empirical maps and theoretical maps, [16]. The empirical maps are the ones that are fitted to the observed flow-pattern database. The theoretical maps are based on prediction from physical models of the flow phenomena. Although attempts are made to develop a generalized flow maps, most of it are only valid for a specific set of conditions and/or fluids. Furthermore, the flow regimes are divided in primary and secondary patterns. The primary pattern denotes the continuous phases while the secondary pattern describes the dispersed
phases within continuous phase. For each secondary pattern a diameter should be assigned in order to determine its interaction with the primary part such as drag. A secondary pattern consisting of different particle sizes, can be modeled by assigning a separate phase for each particle diameter. Figure 2.3 demonstrates a flow regime map from an experiment for the two-phase (air-water) mixture in a vertical pipe with a diameter of 25 [mm], adapted from Weisman [5]. The transition regions observed from the experiments are hatched in the figure.

2.1.2 Basic parameters and Dimensionless numbers

There certain definitions and dimensionless numbers that are handy to have in a toolbox in order to understand the nature of two-phase flows.

Volume fraction

The volume fraction $\alpha_i$ indicates the proportion of phase $i$ in a cell over total volume of the cell as described by (2.1). The value of $\alpha_i$ is strictly bounded, $0 \leq \alpha_i \leq 1$. For a situation of $n$ fluids, there are $n-1$ volume fractions are required for completeness of the model. Hence, $\sum_{j=1}^{n} V_j = V$, $\sum_{i=1}^{n} \alpha_i = 1$.

$$\alpha_i = \frac{V_i}{\sum_{j=1}^{n} V_j},$$

(2.1)

with,
2.1 Multiphase Flows

- $\alpha_i$ volume fraction of the $i$th phase,
- $V_i$ volume of the $i$th phase in a cell in $[m^3]$,
- $\sum_{j=1}^{n} V_j$ the sum of partial volume, which is equal to total volume $V$ in $[m^3]$.

Velocities

The superficial velocity $U_{si}$ is a hypothetical flow velocity of the $i$th phase if the $i$th phase was the only one flowing or present in a given total cross-sectional vector area $A$, as defined in (2.2). It is calculated by dividing the $i$th phase total throughput $Q_i$, volume flow rate of the $i$th phase, by the total cross-sectional vector area $A$.

$$U_{si} = \frac{Q_i}{A}, \quad (2.2)$$

with,

- $U_{si}$: superficial velocity (vector) in $[m s^{-1}]$,
- $Q_i$: volume flow rate of the $i$th phase in $[m^3 s^{-1}]$,
- $A$: total cross-sectional vector area (or surface) in $[m^2]$. The vector area $A$ is product of magnitude of the area $A$ through which the volume $Q_i$ passes and a unit vector normal to the area $n$, $A = An$.

The mixture velocity is expressed as (2.3), which is sum of all superficial velocities. Where $n$ denotes the total number of phases.

$$U_{mix} = \sum_{j=1}^{n} U_{sj}, \quad (2.3)$$

The actual velocity can be determined in analogous way as described in (2.2), but instead of dividing by total cross sectional area $A$ it should be divided by cross sectional area $A_i$ of the corresponding phase. Furthermore, the ideal situation is when the ensemble of two phases is moving simultaneously, as a homogeneous flow. In such a case, the slip ratio is, by definition, taken to be unity (no slip). However, from experimental studies it is observed that it is not the case. Therefore, the slip ratio from (2.4) and slip velocity from (2.5) should be taken into consideration.

$$S = \frac{U_{air}}{U_{water}}, \quad (2.4)$$

$$U_{slip} = |U_{air} - U_{water}|, \quad (2.5)$$

with,

- $U_{slip}$: slip velocity in $[m s^{-1}]$,
- $U_{air}$: velocity of phase air in $[m s^{-1}]$,
- $U_{water}$ total velocity of phase water in $[m s^{-1}]$. 

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Slip effect

Assume an air-water two-phase flows in a pipe domain with cross sectional area $A$. The water hold-up fraction $\gamma_{\text{water}}$ and air void fraction $\gamma_{\text{air}}$ are then defined by (2.6) and (2.7), respectively.

\[
\gamma_{\text{water}} = \frac{A_{\text{water}}}{A}, \quad (2.6)
\]

\[
\gamma_{\text{air}} = \frac{A_{\text{air}}}{A}, \quad (2.7)
\]

with, $A_{\text{water}}$ and $A_{\text{air}}$ being the cross sections occupied by water and air fraction $[m^2]$, respectively. In the pipe flow, the water volume fraction is usually denoted as the fraction of the total volumetric flow rate that consists of liquid. The water hold-up describes the water volume fraction only under conditions of no-slip. This means that the flow is homogeneous and two phases have the same velocity. If no-slip conditions is true, only then the air volume fraction from (2.1), with $i = \text{air}$, is equal to the air void fraction from (2.7). In case no-slip condition are not valid, the velocity of the water hold-up is much larger than the water volume fraction. In that case usefully the air void fraction is smaller than the air volume fraction. The superficial velocity is product of volume fraction and phase velocity as described by (2.8).

\[
U_{si} = \alpha_i U_i \quad (2.8)
\]

Surface tension

Surface tension is the natural behavior that is present along an interface between air and water. Both phases naturally modify their shape accordingly when a physical parameter changes in order to adapt to environment. Both fluid undergo a disorder on a molecular level. In this process water reforms to a stable shape while air does not. This is because the attraction between water molecules are much stronger, due to fact that water is more dense, compared to air. The water molecules in the middle attract other molecules from surrounding while being attracted by other molecules simultaneously. Assuming that water is in the lower level and air is in the upper level. The water molecules at the surface have less water molecules around them, hence those molecules are only attracted towards the lower level. This leads to unfavorable energy state that induces a net tension. The sum of all tensions of all molecules on the surface per unit area is called surface tension. This parameter ensures water to take a stable shape by minimizing the surface area as such that the internal energy is minimized in the system [17]. The molecule disorder is result of the pressure difference across the interface of air and water, which is proportional to the mean curvature as it described by the Young-Laplace equation shown in (2.9).

\[
\Delta p_{\text{air} \rightarrow \text{water}} = \sigma \nabla \cdot n_{\text{water} \rightarrow \text{air}} = \sigma \left( \frac{1}{R_1} + \frac{1}{R_2} \right), \quad (2.9)
\]

where,
2.1 Multiphase Flows

- $\sigma$: surface tension coefficient $[Nm^{-1}]$,
- $n_{water\rightarrow air}$: unit normal pointing towards the gas phase [-],
- $R_1$: first characteristic radius of curvature $[m]$,
- $R_2$: second characteristic radius of curvature $[m]$.

Furthermore, due to presence of surface tension forces and differences in material properties at the interface the viscosity will change. This leads to jumps and discontinuities for pressure and the gradient of the velocity field at the interface, [18]. For better understanding of this situation one should identify the dominant forces acting on the flow. To compare these forces in a proper way use can be made of dimensionless analysis. In this subsection some of the dimensionless number relevant to this project are presented. The characteristic length in this report is denoted by a diameter $D$ of a pipe.

**Reynolds number** is the ratio of the inertial and the viscous forces, which is defined as following:

$$Re = \frac{\rho UD}{\mu} = \frac{UD}{\nu}, \quad (2.10)$$

where,

- $\rho$: the density of the fluid in $[kgm^{-3}]$,
- $U$: the velocity of the fluid in $[ms^{-1}]$,
- $D$: the diameter of the pipe in $[m]$,
- $\mu$: the dynamic viscosity of the fluid in $[kgm^{-1}s^{-1}]$,
- $\nu$: the kinematic viscosity of the fluid in $[m^2s^{-1}]$.

Reynolds number is used to predict flow patterns in different fluid flow cases.

**Froude number** is the ratio of the inertial and the gravitational forces, or the ratio of the kinetic and potential energies of the air or the water and it is defined as follows:

$$Fr = \frac{U}{\sqrt{gD}}, \quad (2.11)$$

with,

- $g$: the gravitational acceleration constant in $[ms^{-2}]$.

Froude number describes the resistance of a partially submerged object moving through water.
**Weber number** expresses the ratio of inertial to surface tension forces (i.e. curvature),

\[ We = \frac{\rho DU^2}{\sigma}, \]  
(2.12)

Weber number is particularly useful for two-phase flows, which can be used to analyze the interface between i.e. air and water.

- \( \sigma \): surface tension coefficient \([Nm^{-1}]\).

**Eotvos number** measuring the relation of gravitational forces to surface tension forces,

\[ Eo = \frac{\rho g D^2}{\sigma}. \]  
(2.13)

**Morton number** this number is expressed as follows,

\[ Mo = \frac{g \mu^4}{\rho^3}. \]  
(2.14)

Morton number together with Eotvos number can be used to characterize the shape of the bubbles or drops moving in a surrounding fluid or continuous phase.

### 2.2 Numerical methodology

This sections presents the numerical methodology that is relevant for the content of this report. The derivations and other detailed informations can be found in several works a.o. [19], [20], [21], [22] and [23], which are considered for this section. In Subsection 2.2.1 the governing equations are shown. The selected frame of reference is presented in Subsection 2.2.2. Subsection 2.2.5 deals with the numerical techniques. The Volume Of Fluid (VOF) method is explained in Subsection 2.2.5. Finally, the solution algorithm and the turbulence are addressed in Subsection 2.2.6 and 2.2.7, respectively.

#### 2.2.1 Governing Equations

The dynamics of the fluid is described by the Navier-Stokes equations. That is a product of conservation of mass from (2.15) and conservation of momentum given in (2.16). It should be noted that conservation of energy is not considered in this case.

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0, \]  
(2.15)

\[ \frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho U U) = -\nabla p + \nabla \cdot \tau + \rho f, \]  
(2.16)
2.2 Numerical methodology

where,

- \( \rho \): density of the fluid in \([kgm^{-3}]\),
- \( t \): time in \([s]\),
- \( \mathbf{U} \): velocity field \([ms^{-1}]\),
- \( p \): pressure in \([kgm^{-1}s^{-2}]\),
- \( \tau \): viscous stress tensor, and
- \( f \): external source, i.e. gravity.

Considering constitutive law for the Newtonian fluids, the viscous stress tensor can be written in terms of material properties as,

\[
\tau = \mu \left[ \nabla \mathbf{U} + (\nabla \mathbf{U})^T - \frac{2}{3} (\nabla \cdot \mathbf{U}) \mathbf{I} \right],
\]

(2.17)

with,

- \( \nu \): kinematic viscosity in \([m^2s^{-1}]\),
- \( \mathbf{I} \): identity matrix, and
- \( \mu \): Dynamic viscosity in \([kgm^{-1}s^{-1}]\).

**Incompressible flow**

For an incompressible case the density remains constant during the motion. Hence, the first term of (2.15) vanishes resulting to (2.18), continuity equation.

\[
\nabla \cdot \mathbf{U} = 0.
\]

(2.18)

Applying (2.18) to viscous stress tensor, the \( \nabla \cdot \mathbf{U} \) term of (2.17) will vanish. Moreover, by assuming that the density and the dynamic viscosity stay constant the conservation of momentum from (2.16) can be rewritten as (2.19).

\[
\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot (\mathbf{U} \mathbf{U}) = -\frac{1}{\rho} \nabla p + \nabla \cdot (\nu \nabla \mathbf{U}) + \mathbf{f},
\]

(2.19)

where, \( \nu = \frac{\mu}{\rho} \) represents the kinematic viscosity. Equations (2.18) and (2.19) describe the Navier-Stokes equations, in the differential form, for incompressible case. These equations have to be solved for three components of the fluid velocity and the fluid pressure to describe the dynamics of a fluid.
2.2.2 Frame of reference

Navier-Stokes equations from (2.19) describes the fluid motion at a point. For the engineering applications it is necessary to simulate a real case scenario, like fluid flow over an airfoil or through a pipe. Therefore, it is important to model the fluid motion behavior for a larger domain than just on a point. There are two approaches for solving the equations over a larger domain, namely the Lagrangian and the Eulerian methods. The difference between these two is the frame of reference. When the Lagrangian methods are applied, the solution point will be moving with the fluid. In other words the reference frame is not fixed but it moves with the observer. Although this approach is found to be relatively easier to set up, the experience learns that there occasionally some problems on the boundaries where constant attention should be paid. The Eulerian method is where the fluid, solution point, is moving through a fixed mesh (reference frame is fixed). This method is relatively easier to formulate and does not require complex treatments on the boundaries. Maybe the best advantage of the latter method is that it is well understood and great amount of applications are reported. The well-known techniques of Eulerian approach are the finite-element, finite difference and finite volume method. Comparing Finite Volume Method (FVM) to other two methods, one of the important aspects of FVM is that the method is based on discretization of the integral form of governing equations over each control volume. Hence, the conservation laws are satisfied at the discrete level. Because of the aforementioned reasons, the Eulerian approach with FVM is selected to proceed with.

2.2.3 Finite volume method

The aim of a numerical method is to transform the set of partial differential equations, such as Navier-Stokes, into an associated system of linear algebraic equations. The solution of that system results to a set of values which corresponds to the solution of the partial differential equations at pre-determined discrete locations in space and time. The discretization procedure of FVM can be divided in three sections, namely discretization of the solution domain (involving the mesh), equation discretization (involving the convection, diffusion and the source term of governing equations) and temporal discretization (involving the temporal derivative of governing equation).

- The discretization of the solution domain provides a numerical recipe for the computational domain and the boundary (mesh). The computational domain includes the positions of solution points at which the governing equations are solved. These points are located in a space that is divided into a finite number of discrete regions that are called control volumes or cells. The procedure for discretization of the solution domain is divided in two subsections, namely:
  - spatial discretization: the computational domain consists of control volumes (CV). A CV is bounded by set of faces, which are either internal face or boundary faces;
  - temporal discretization: for this discretization it is enough to prescribe the size of the time-step that will be used during the calculations.
• Equation discretization provides recipe to transform the terms of governing equations into algebraic expression. To this end the terms from governing equations are solved by integrating over control volume. The Gauss divergence theorem is used to transform the divergence terms in the governing equations into surface integrals over the volume’s boundary. Accordingly, these surface integrals are determined as the sum of the values on the cell faces. The velocity field $U$ from the surface integrals is stored at the cell centers. In order to determine the surface integrals for convection and diffusion terms the $U$ should be evaluated at the cell faces. This is done by a convection differencing schemes. One of these is Central Differencing (CD) scheme where the face value is computed by assuming a linear variation of the interpolated $U$ between two neighboring cells to face. It has been shown that for convection-dominated problems, which is the subject of current project, the CD schemes causes unphysical oscillations in the solution, [21] and [20]. A different technique is the upwind differencing (UD) scheme where the face value of velocity field $U$ is determined by considering the value of the cell center in the upstream direction. The discretization of the source term is done by first linearizing it and afterwards the volume integral is determined. A general formulation for the treatment of the source term is provided by Patankar in [20].

• Temporal discretization is necessary in case of transient simulation. In that case the time interval is divided into number of time-steps. The time integrals are solved by using the implicit Euler, explicit Euler or combination of both Crank-Nicolson schemes. In part 1 of this project use is made of implicit Euler (Backward Euler) scheme. In part 2 of this project a different approach is applied for temporal discretization. That is based on second order Runge-Kutta scheme and the essentials will be introduced in the next subsection.

2.2.4 Singly diagonal implicit Runge-Kutta (SDIRK)

In the part 2 of this project use is made of second order Runge-Kutta method for temporal discretization technique. The essentials of this technique are described here shortly. Assume (2.20) for the initial value problem,

$$\frac{\partial y}{\partial t} = f(t, y), \quad \text{and} \quad y_0(t_0) = y_0.$$  \hspace{1cm} (2.20)

Then the second order Runge-Kutta method is evaluated as follow,

$$y_1 = y_0 + \Delta t \left(b_1 k_1 + b_2 k_2\right),$$  \hspace{1cm} (2.21)

with, $k_1$ and $k_2$ given in (2.22) and ((2.23)), respectively.

$$k_1 = f(t_0 + c_1 \Delta t, y_0 + \Delta t a_{11} k_1)$$  \hspace{1cm} (2.22)

$$k_2 = f(t_0 + c_2 \Delta t, y_0 + \Delta t (a_{21} k_1 + a_{22} k_2))$$  \hspace{1cm} (2.23)

The coefficients $a$, $b$ and $c$ are real and they are ranked in a so called Butcher tableau [24], which forms the basis of the the Runge-Kutta schemes. For the second order Runge-Kutta
Butcher tableau equals to scheme that is presented by Ascher et al. [25], (2.24). This scheme is used for temporal discretization.

\[
\begin{array}{c|cc}
 c_1 & a_{11} & a_{21} \\
 c_2 & a_{22} & b_2 \\
 b_1 & & \\
\end{array} \quad = \quad \begin{array}{c|cc}
 \gamma & & \\
 1 & 1-\gamma & \gamma \\
 1-\gamma & \gamma & \\
\end{array},
\]  

(2.24)

where, \( \gamma = 1 - \sqrt{2}/2 \) that also know as singly diagonal implicit Runge-Kutta (SDIRK) scheme.

### 2.2.5 Volume of fluid method

Volume Of Fluid method (VOF) was developed by Hirt et al. [26] for multiphase flow simulations. In this project the VOF based solver \texttt{interFoam} from OpenFOAM is used. VOF is an interface capturing method, which relies on the indicator function. This function provide information about occupation of a cell, whether it is filled by one fluid or another, or a mix of both. The indicator function represents the volume fraction of one phase and its transport equation is given by (2.25).

\[
\frac{\partial \alpha}{\partial t} + \nabla \cdot (U \alpha) = 0,
\]  

(2.25)

where,

- \( \alpha \): volume fraction, which takes value \( \alpha = 0 \) for air, \( \alpha = 1 \) for water and \( 0 \leq \alpha \leq 1 \) for a mix composition,

Equation (2.25) forms together with continuity and momentum equations from (2.18) and (2.19), respectively, the governing equations for VOF method. To this end a couple of items should be emphasized as done in the following bullet points:

- the two fluids are in-miscible and there exists a clear interface between them,
- the gradients of the phase fraction from (2.25) are taken into consideration only in the interface region,
- the body force \( f \) from (2.19) includes gravity force \( f_g \) and surface tension force \( f_\sigma \) which effects the interface,
- furthermore, the physical properties are represented by weighted averages of liquid volume fraction. This means that a property equals the property of the fluid that occupies that cell and only varies across the interface. This idea is described by mixture properties from (2.26) and (2.27) for density and dynamic viscosity, respectively.

\[
\rho = \rho_W \alpha + \rho_A (1 - \alpha),
\]  

(2.26)
\[ \mu = \mu_W \alpha + \mu_A (1 - \alpha). \] (2.27)

Due to surface tension at the water-air interface an additional pressure gradient is generated. This is represented as a surface force per unite volume in (2.29) using continuum surface force formulation from Brackbill et al. [27].

\[ \mathbf{f}_\sigma = \sigma \kappa \nabla \alpha, \] (2.28)

with,

- \( \sigma \): surface tension that has a constant value in \([Nm^{-1}]\),
- \( \kappa \): mean curvature of the free surface given in (2.29),

\[ \kappa = -\nabla \cdot \left( \frac{\nabla \alpha}{|\nabla \alpha|} \right). \] (2.29)

Moreover, the surface tension term in momentum equation adds numerical instabilities and/or numerical noise along poor representation of capillary effects. This problem is manifested as so called spurious currents in the flow field of the numerical simulations, [28].

### 2.2.6 Solution algorithm

In this project is the Pressure Implicit with Splitting of Operators (PISO) algorithm is used that was published by Issa [29]. This algorithm is used for pressure-velocity coupling in transient calculations. In this subsection it will be introduced shortly, for detailed explanation one may study [19], [23] and [22]. In case of SDIRK, the steps are pointed out by Frederix et al. in [2]. In the standard PISO algorithm each time-step is solved through the following three steps:

1. For a best guess pressure field the momentum equations are solved for velocity field.
2. The velocity field obtained from previous step is used to solve the pressure equation.
3. Subsequently, the obtained pressures from previous step are used to correct the velocity field.

Only for steps 2 and 3 an iteration is required. A priori PISO algorithm, within each time step, additional equations are solved for multi-phase flow. The turbulence models are solved afterwards. A nice transient solution procedure PISO loop for incompressible turbulent flows is given by Jasak in [19].
2.2.7 Turbulence

Above a certain Reynolds number any flow, single-phase and multiphase, becomes turbulent. In a turbulent process a chaotic and random state of motion will develop. In that process the velocity and pressure change continuously with time. Most of the flows in the engineering applications are turbulent flows. Hence, it is necessary to take turbulence into consideration. Moreover, analyzing turbulence behavior for single-phase flows is complex and still considered as a not resolved issue in science. However, comparing to two-phase flows, it has been studied extensively and there are several reliable models available. Modeling turbulence behavior for multiphase cases is even more complex because of the nature of multiphase flows itself. Currently the knowledge about turbulence, modeling within the multiphase framework, is very limited. The models are far from a final robust and mathematical description. The existing models are derived from single-phase models. Furthermore those are strictly case dependent and often not very accurate. For example for models meant for bubbly flow regime, the turbulent kinetic energy of gas phases is usefully neglected because of large density differences between gas and liquid phases, [7, 30, 6]. Brauner et al. demonstrated that the momentum transfer at the interface was considered to be the crucial issue in modeling of two-phase (gas-liquid) stratified flows [31]. Furthermore, in two-phase flows beside the natural turbulence also the disturbance created by the bubbles in the fluid should be taken into account. This chapter provides some fundamental information on turbulence phenomena that is applicable for single-phase and two-phase flows.

Energy cascade

Turbulence is a three dimensional process which consists of rotational flow structures. These structures are called turbulent eddies with a wide range of length scales. The larger eddies provide the smaller eddies the kinetic energy, as described by process called energy cascade. Figure 2.4 shows a typical energy spectrum for turbulent flow versus wavenumber \( \kappa \) in a \( \log - \log \) representation. The energy spectrum \( E(\kappa) \) describes the energy contained in the eddies with length scale size \( l \) from (2.30) and wavenumber \( \kappa \).

\[
  l = \frac{1}{\kappa}. \tag{2.30}
\]

The turbulent kinetic energy is expressed by (2.31).

\[
  k = \int_{\kappa_1}^{\kappa_2} E(\kappa) \, d\kappa. \tag{2.31}
\]

Figure 2.4 can be divided in three ranges of turbulent scales, namely large scale range, inertial subrange and dissipation range.

- Large scale range (\( \kappa \to 0 \)): this is where the energy is produced. This range is dominated by turbulent kinetic energy \( k \), which is proportional to \( 1/l \), and turbulence dissipation rate \( \varepsilon \). From Figure 2.4 it can be observed that eddies with the largest length scale contains most of the turbulent kinetic energy. For modeling of any turbulent flow this range is necessary to be taken into account.
2.2 Numerical methodology

- Inertial subrange: this is where the energy is transferred. This range is dominated by \( \kappa \) and \( \varepsilon \). For sufficiently high Reynolds number, this is an intermediate scale range between the large and the smallest scales. Through dimensional analysis it can be shown that \( E(\kappa) \propto \kappa^{-5/3} \), which is known as Kolmogorov -5/3 law.

- Dissipation range (\( \kappa \to 1/\eta \)): this is where the turbulence is destroyed and transformed into heat. In this range the behavior of eddies is dictated by the viscosity \( \nu \) and turbulence dissipation rate \( \varepsilon \), which is the rate of energy transferred from the large scales. This range has the lowest kinetic energies while having highest wavenumbers. The smallest eddies are represented by Kolmogorov scales (\( \eta \)) and are indicative of the scales at which the dissipation occurs.

![Figure 2.4: Schematic representation of turbulence spectrum in log – log scales described by RANS, LES, and DNS approaches. Adapted from [7].](image)

**Approaches**

There are three approaches to simulate or model the turbulence behaviors, namely the Direct Numerical Simulation (DNS), Large Eddy Simulations (LES) and Reynolds averaged Navier-Stokes (RANS). Figure 2.5 shows a representation of all three approaches for a flow over a cylinder. As can be seen DNS is the most accurate one since it resolves all scales in the flow. However, due to mesh resolution and time step size the demand on computational resources are very high. Therefore, DNS is not feasible for industrial and engineering applications. In LES, as the name says, the large eddies are resolved while small scales, sub-grid scales, are modeled. The computational cost of LES is less than DNS but higher than RANS. RANS models do not require very fine mesh, hence it demands less from computational resources. Therefore, it is very popular within the industrial and engineering community. In the current project attention is paid to RANS models. As can be observed from Figure 2.4, the eddies with highest kinetic energy can be modeled by the RANS techniques (no dynamics i.e., just an integral length-scale). The intermediate part is partially simulated and partially modeled using LES technique (dynamics of the most energetic eddies). DNS resolves all scales (the dynamics of all the eddies).
RANS equations

A turbulent flow means a state of continuous instability. In this state the fluctuation of the flow \( f'(x,t) \) can be separated from the mean of the flow \( \bar{f}(x,t) \). This is done by decomposing the main variables from Navier-Stokes equations by applying the Reynolds averaging technique from (2.32).

\[
f(x,t) = \bar{f}(x,t) + f'(x,t),
\]

(2.32)

where, \( x \) is the position vector and \( t \) the time. The mean component is given as,

\[
\bar{f}(x,t) = \lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} f_k(x,t),
\]

(2.33)

where, \( f_k \) are the samples of \( f \) and \( k = 1, 2, 3, ..., N \) is the number of samples. Averaging the governing equations from (2.18) and (2.19) it results to Reynolds averaged Navier-Stokes (RANS) equations in tensor form as given in (2.34) and (2.35).

\[
\frac{\partial U_i}{\partial x_i} = 0,
\]

(2.34)

\[
\rho \frac{\partial U_i}{\partial t} + \rho \frac{\partial}{\partial x_j} (U_i U_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( 2\mu S_{ij} - \rho \left( U'_i U'_j \right) \right),
\]

(2.35)

where, \( S_{ij} \) denotes the mean strain-rate tensor given in (2.36).

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)
\]

(2.36)

By the application of (2.34) and substitution of (2.36), Equation (2.35) can be expressed as,

\[
\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_i \partial x_j} - \frac{\partial U_i U'_j}{\partial x_j}.
\]

(2.37)
It can be seen that due to averaging an additional term is generated, $-\rho \left( \overline{U'_iU'_j} \right)$. This term is called the Reynolds stress tensor term that acts as an extra stress term. With this term the number of unknown variables are increased while the number of equations stayed the same. This leads to the turbulence closure problem since there are not enough equations to solve for the unknown variables. Quantification of this term is not an easy task since the small turbulent flows that induce it cannot be directly modeled. One of the popular approaches that is used in this project is the so called Boussinesq hypothesis. In this approach approximation is done to treat the Reynolds stress term similarly as the conventional stress term (2.17) and to model it using viscosity. This called the eddy viscosity modeling concept. Hence,

$$-\overline{U'_iU'_j} = 2\nu_t S_{ij} - \frac{2}{3}k\delta_{ij},$$  \hspace{1cm} (2.38)

where,

- $\delta_{ij}$: Kronecker Delta,
- $k = \frac{1}{2} \overline{U'^2} = \frac{1}{2} \overline{U'_iU'_i}$; the turbulent kinetic energy, and
- $\nu_t$: the eddy or turbulent viscosity, which is assumed as an isotropic scalar quantity.

Equation (2.38) replaces the Reynolds stresses by introducing two new unknowns, $k$ and $\nu_t$. These new quantities vary from point to point in the flow. The most popular approach is to express the $\nu_t$ in terms of turbulent kinetic energy $k$ and its dissipation rate $\varepsilon$ ($k - \varepsilon$ Model) or its specific rate of dissipation $\omega$ ($k - \omega$ Model). These are popular two-equation models that are used in this project.

**Standard $k - \varepsilon$ Model**

This is a two equation model that parametrizes the turbulence problem into two variables, $k$ and $\varepsilon$. Where $k$ is representing the turbulent kinetic energy and $\varepsilon$ the turbulent dissipation rate. Both parameters have their own convection-diffusion equation. In this model the eddy viscosity is determined by (2.39), as shown in [32],

$$\nu_t = C_\mu \frac{k^2}{\varepsilon},$$  \hspace{1cm} (2.39)

where, $C_\mu$ denotes a constant of the $k - \varepsilon$ model that equals to 0.09 [33].

**$k - \omega$ Model**

The $k - \omega$ model, is similar to $k - \varepsilon$ in many aspects. The difference is the turbulent dissipation rate $\omega$. In this model the eddy viscosity is determined by (2.40) as shown in [33],

$$\nu_t = \frac{k}{\omega},$$  \hspace{1cm} (2.40)
$k - \omega$ SST Model

This is a hybrid model that uses a transformation of the standard $k - \varepsilon$ into a $k - \omega$ model in the near-wall region and the standard $k - \varepsilon$ in the fully turbulent region far from the wall, as reported in [34]. The Reynolds stress computation and $k$-equation are the same as previous two models. But the $\varepsilon$-equation is transformed into an $\omega$ ($\varepsilon = k\omega$). In this model the eddy viscosity is determined as its shown in [34].

**Estimation of $k$, $\varepsilon$ and $\omega$**

The flows in this project are considered as low-turbulence. The initial values for the $k$, $\varepsilon$ and $\omega$ are estimated by (2.41)-(2.43).

$$k \approx 1.5I^2U^2,$$  \hspace{1cm} (2.41)

$$\varepsilon \approx C_\mu \frac{k^{1.5}}{0.38D},$$  \hspace{1cm} (2.42)

$$\omega \approx C_\mu^{-\frac{1}{4}} \frac{k^{0.5}}{0.38D},$$  \hspace{1cm} (2.43)

with, $I$ representing the initial turbulence intensity that is commonly assumed to be 5% and $D$ representing the diameter of the pipe.

**Near-wall region treatment**

The velocity profile can be divided into two regions, an inner region representing $\approx 1\%$ of free stream velocity and an outer region representing the rest of the free stream velocity. Accordingly, the inner region can be divided in three layers namely, the laminar or viscous sublayer, the buffer layer and the turbulent zone. The laminar sublayer is adjacent to the wall. Turbulent zone forms together with outer region the so called turbulent core. In order to resolve all the details near the wall, the mesh needs to be very fine in the inner region. For meshing one can use than the law-of-the-wall tool, which assumes that the turbulence of a local near-wall region is a function only of the flow conditions associated to that local near-wall region. Hence, those conditions are independent from the flow conditions further away. The law-of-the-wall covers the three inner layers. However, since the gradients are very steep near the wall and a fine mesh needs significant computational effort it is usually impractical to resolve all the details of the flow in the near-wall region. Instead of resolving, wall-function boundary conditions can be used.

**Wall-functions**

The wall-functions are derived from a semi-empirical model of turbulent boundary layer flow the law-of-the-wall, [32]. These functions represent a simplified model of turbulence, that describes the near-wall physics of the velocity, the turbulent kinetic energy $k$ and the dissipation...
2.3 Modeling slug flows in vertical pipe

From previous chapters it has become evident that multiphase flows have a complex nature. Modeling all the regimes present in multiphase flows is outside the Scope of the current project. From the objective as mentioned in the introduction of this report, the main focus lies on CFD of stratified (co-current) flows in a vertical pipe for NRS scenarios. Stratified flows are characterized by large interfaces between two phases, i.e. air/water. A multiphase regime that is related to stratified flows is slug flow. Slug flows in motion through a fluid with surface tension evolve to a particular sort bubble flows, namely Taylor bubble flows. This chapter is divided in two sections. The physics of Taylor bubble flows are introduced in Section 2.3.1. The state-of-the-art modeling of this regime is presented in Section 2.3.2.

2.3.1 Taylor bubble

As it is explained in the previous chapter, slug flows are characterized by large gas pockets in the continuous liquid having large interfaces [6, 16]. Slug flows have enormous similarities to plug flows, the main differences are that slug flows are generally bigger in size and move relatively faster. Furthermore, the topology of the slug flows depend from their dynamics. Usually, slug flows in a vertical pipe are called Taylor bubble flows. These bubbles are named after G.I. Taylor who was co-writer of the study: The mechanics of large bubble rising through liquids and through liquids in tubes, [35]. The main characteristic that makes these bubbles a unique group within the slug flows is their morphology. A Taylor bubble is recognized by their bullet shaped head, as shown in Figures 2.1 and 2.2, under the class slug regime. There are three important parameters that characterize Taylor bubble flows, namely the bubble rise velocity [36, 37, 38], the thickness of the falling liquid film between the bubble and the pipe wall [39] and the wake of the bubble [37, 40]. The film region and the near the wake region are illustrated by Figure 2.6. In this figure an image is taken from Taylor bubble’s tail from the experiment measurements presented in [9]. The slug flows are evolved to Taylor bubble flows due to bubble rise velocity and surface tension in a pipe with a certain diameter. Furthermore, in a pipe with relatively larger diameters there are some entrainment of air from the Taylor bubble into the water slug region. While in the pipes with smaller diameters this is not the case. It is reported by various authors that slug flows can not be created when the diameter of the pipe is larger than certain value [41, 42, 43, 44]. Besides, the geometry of the pipe, the orientation of the pipe has also significant influences on the flow components [45]. Moreover, the volume of slug in the liquid region is proportional to the diameter of the pipe [46]. In the vertical pipe isolated Taylor bubble rises almost uniformly. The falling film, penetrates the bubble from the rear side with the possibility of creating a recirculation region.
2.3.2 Literature review

The main challenges for predicting multiphase flows is the transfer rates of mass, momentum, energy and turbulence process in the interface between the two phases [50]. The morphology of the structures as can been seen from Figure 2.2 are very sensitive to these processes [51].

In the early days, modeling of slug flow was primely based on studies carried out by Dumitrescu [11] and by Davies et al. [35]. The main focus of those studies was on the rise velocity of a single very long Taylor bubble flows in a stagnant liquid. Nicklin et al. [52], demonstrated that the Taylor bubble rise velocity does not depend on its length. Furthermore, he proposed an empirical relationship which describes the rise velocity of a Taylor bubble in a stagnant water column. The first comprehensive model was presented by Fernandes et al., in which he predicted the average void fraction, the velocity of the Taylor bubble, the translation velocity of the Taylor bubble, the mean velocity of the falling film and the pressure gradient [53]. Also Orell et al.,[54], developed a model that has similarities in most aspects to the model developed by Fernandes et al. Dukler et al. pointed out conditions for
the existence of the slug flow pattern in [55]. In more recent days extensive studies are carried out for purpose of slug flows and models are proposed for fully developed flows [56, 31, 53, 38]. For empirical relations a review is presented on vertical gas-liquid slug flows by Morgado et al. [47]. In this study the mechanisms inside the Taylor bubble are extensively studied by using the capabilities of dimensional analysis. On the other hand models are presented for describing flow pattern transitions during steady gas-liquid flow in vertical pipes, based on physical mechanisms suggested for each transition by Taitel et al. in [57, 58]. These models includes the effect of fluid properties and pipe geometry, hence free of the limitations of empirically based transition maps or correlations. The rise velocity of a Taylor bubble is influenced by gravitational, viscous, inertial and interfacial forces. Therefore, it is sufficient to work with $Fr = (Eo, Mo)$ for modeling the rise of a Taylor bubble in a stagnant liquid column as reported in [49, 59, 38]. Alexander et al. simulated Taylor flow in intermediate diameter channels using VOF for laminar and turbulent conditions as presented in [60]. Aland et al. presented a quantitative comparison of Taylor flow simulations conducted in 2D and 3D. [61]. They compared a sharp-interface model based on a moving grid aligned with the bubble boundary and a diffuse-interface model where the bubble shape is implicitly given by a phase-field function. Although most of the simulations are performed in Finite Volume Method, Edvinsson et al. conducted an analysis of Taylor flow using Finite Element techniques [62]. For this study a moving surface formulation is used to predicted the bubble shape. Behafarid et al. carried out a DNS study on large bubble motion and liquid film in vertical pipes and inclined narrow channels using a FEM based solver as presented in [63]. A modified Level-Set Method (LSM) used to capture the liquid/gas interface.

Considering turbulence in stratified two-phase flows with large interfaces. Most of the simulations are LES/DNS based studies, [64, 65, 66]. However, DNS is not cost worthy specially in cases with high Reynolds number due to demand on the computational resources. Currently, LES is the common method for modeling turbulent stratified pipe flows. The popular standard RANS models for modeling of single-phase flow fail to predict turbulence in case of stratified flows with large interfaces.

In the study [67], the turbulence behavior of the interface in stratified flow is modeled using classical RANS models. In that study the turbulence near the gas side of the interface is assumed to be equivalent to turbulence near the wall as proposed by studies [64, 65]. The concluding remarks from this study was that there are no optimum and robust methods that are capable to model the turbulent behavior at the interface. The limitation of RANS models, for similar two-phase purposes, are also pointed out by Lamarque et al. in [68]. In that study the results from RANS modeling ware compared to LES results. In different studies that are carried out by Hohne et al. the disagreement between classical RANS models with the experimental measurements are demonstrated [69, 70].

For the simulations of the stratified flows where large scale interfaces, i.e. Taylor bubble, are present the classical RANS models breaks down. This happens because near the interface the turbulent viscosity $\nu_t$ is over predicted. A high velocity gradient at the interface between two fluids results in generation of high turbulent viscosity ($\nu_t$), in both phases. The turbulent viscosity is included in the RANS models, that are used for modeling the turbulent behaviors of the flow. To address this issue Egorov developed a model which damps the high value of the $\nu_t$.
turbulent viscosity in the interface, [3]. Moreover, he suggested that at a large-scale interface
the lighter phase may see the heavier phase as a solid wall. Hence, a wall-like treatment of
turbulent dissipation at the interface should be applied. This is done by forcing the specific
turbulence dissipation \( \omega \) to a wall like value as shown in (2.44).

\[
\omega_{int}^i = B \frac{6\nu_i}{\beta \Delta x^2},  
\]

(2.44)

with,

- \( B \): non-dimensional coefficient, mesh dependent,
- \( \nu_i \): kinematic viscosity of the \( i \)th phase,
- \( \beta \): \( k - \omega \) closure coefficient of destruction term, which is equal to 0.075, and
- \( \Delta x^2 \): typical computational cell size near the interface.

The value of \( \omega_{int}^i \) is inserted in the vicinity of the interface by introducing (2.45) as a source
term to \( \omega_i \) transport equation.

\[
S_{int}^i = A \alpha_i \rho_i \beta \left( \omega_{int}^i \right)^2,  
\]

(2.45)

with,

- \( A = |\Delta \alpha| \Delta x \): interfacial area density,
- \( \alpha_i \): the volume friction of the \( i \)th phase, and
- \( \rho_i \): density of the \( i \)th phase.

The factor \( A \) in (2.45) activates the source term only at the free surface while it cancels
the standard destruction term of the RANS model. Hence, it damps the high value of the
turbulence model at the interface. It has been reported that the non-dimensional Egorov
model coefficient is grid dependent, [4]. A modified version of Egorov term is formulated by
Frederix et al. in [4], in which consistent results are obtained for different grids comparing to
the original formulation of the Egorov model. Frederix represents the inter-facial dissipation
rate \( \omega_{int}^i \) in terms of a length scale \( \delta \) i. e.,

\[
\omega_{int,s}^i = \frac{\nu_i}{\beta \delta^2}.  
\]

(2.46)

The length scale \( \delta \) is related to \( B \) as,

\[
\delta^2 = \frac{\Delta x^2}{6B}.  
\]

(2.47)

Hence, by applying the inter-facial dissipation rate from (2.46) into the source term it will
avoid the inconvenient computations of the mesh dependent selection of \( B \). This tool makes
it computationally possible to link the turbulent core to the physical boundary condition at
the wall of the domain.
2.4 CFD tool OpenFOAM

In this project the simulations are performed by using the OpenFOAM- based VOF solver interFoam, version 4.1. OpenFOAM is a C++ library that contains source code for solver and utilities. A case is set-up using the case folder which consists of three root directories namely,

1. **system**, contains the files where the information about meshing and the numerical methodology are saved. Some of these files are summed as follows,
   - `blockMeshDict`: where mesh and boundaries of the domain are defined
   - `controlDict`: containing information about about the time step, solver etc.
   - `funkySetFieldsDict`: this is an external utilities, which is used to insert the bubble
   - `fvSchemes`: where the differential schemes are selected
   - `fvSolutions`: file where solvers and used algorithms are selected and tuned

2. **constant**, contains o.a. the flow transport and turbulence properties.

3. 0-directory, in the zero directory are the initial conditions for velocity, pressure, phase fraction and turbulence related quantities are saved.

Furthermore, OpenFOAM has a disadvantage of lacking of proper user manuals for the solvers. This makes the learning very steep and time consuming. The main advantage is that it is open source hence, very attractive for industrial applications.

Next chapter deals with 2D Taylor bubble morphology validation.
Chapter 3

2D Taylor bubble morphology validation

3.1 Introduction

This chapter is about Taylor Bubble morphology validation in a vertical pipe. The analytical model of Tomiyama et al. [1] is selected as the data set for the validation. The procedure of validation is as follows. Firstly, the computational domain, the boundary conditions, the initial condition and the flow properties are implemented into OpenFOAM. Secondly, the calculations are done with VOF based solver, interFOAM. Subsequently, the produced results are post-processed and compared with the analytical approach as formulated by Tomiyama et al. This chapter deals with first four items of Part 1 of the research objective as pointed out in Section 1.2. At the end of this chapter the following questions should be answered:

- is interFOAM in combination with a RANS model able to predict Taylor bubble morphology adequately?
- what are the appropriate boundary and initial conditions?
- is the grid in-dependence achieved?

Accordingly, this chapter is structured as follows. The details of the selected data set are presented in Section 3.2. Section 3.3 is devoted to numerical setup in which the computational domain, the boundary conditions, the initial conditions, the numerical schemes, the thermo-physical properties and the mesh. This will be followed by Section 3.4, where based on the simulation results an appropriate initial and boundary condition is selected. Also, in Section 3.4 the transient behavior of the bubble is analyzed and a grid dependency study is presented. The Section 3.5 finalizes this chapter with a conclusion.
3.2 Analytical approach of Tomiyama et al. [1]

In Tomiyama’s study an analytical approach is presented that describes the morphology of a rising bubble. In other words, the model predicts the interface of a bubble. The bubbles are characterized by a radius ratio $\lambda$ represented by (3.1),

$$\lambda = \frac{r_s}{r_p},$$

(3.1)

with,

- $r_s$: the hypothetical radius of the spherical bubble in [m], and
- $r_p$: the radius of the pipe in [m].

For Taylor bubble it is required that $\lambda \geq 1.4$, which means that the diameter of the bubble is larger than the diameter of the pipe. Hence, the radius of the spherical bubble is a hypothetical radius. The analytical model of Tomiyama et al. is represented by (3.2) - (3.5). In that model, the shape of the bubble is in function of Reynolds number with characteristic length that is equal to $D_p$ and velocity that is equal to mean flow velocity $V_W$. Figure 3.1 shows three bubbles with three different $\lambda$’s as described by Tomiyama et. al [1]. The interface of the bubbles are compared with the analytical model, (3.2), that is represented in Figure 3.1 by circles. Comparing the three bubbles from Figure 3.1, it can be noted that the interface of a bubble is independent of $\lambda$. However, $\lambda$ does affect the length and hence, thus the volume of the bubble that will be determined in Section A. Hence, for morphology validation only a part of the Taylor bubble is enough to compare with analytical model. The shape function from (3.2) is plotted in Figure 3.2 that corresponds with the red-dashed-square from Figure 3.1. Contrary to Figure 3.1, the axes in Figure 3.2 are the other way around. The horizontal axis of Figure 3.2 is placed along the centerline of the pipe while the vertical axis represents the radial direction. Similarly to Figure 3.1, both axes are normalized by the pipe radius, $r_p$. The results from the simulation will be compared to Figure 3.2 in Section 3.4. Furthermore, the other dimensions of the pipe are compatible to [1]. The diameter of the pipe ($D_p$) is 24.8 millimeters and the length of the pipe ($L_p$) is set to be 1.0 meter. The mean flow velocity ($V_W$) is 1.0 [ms$^{-1}$]. These parameters will be used throughout this chapter and are added in Table 3.1.

$$R(Z) = 0.9 - \left[Z^{0.70} + 0.91/A \right]^{1/A},$$

(3.2)

$$R = \frac{r}{r_p},$$

(3.3)

$$Z = \frac{z}{r_p},$$

(3.4)

$$A = \min \left(3.26 \cdot 10^4 \cdot Re_W - 2.83, \quad 2.29 \cdot 10^5 \cdot Re_W - 2.36 \right),$$

(3.5)

where,
3.2 Analytical approach of Tomiyama et al. [1]

- $\mathcal{R}$: the normalized shape function with respect to pipe radius $r_p$,
- $Z$: the normalized cylindrical coordinate with respect to pipe radius $r_p$,
- $A$: bubble shape coefficient expressed in (3.1),
- $z$: cylindrical coordinate in [m], and
- $Re_W$: Reynolds number of water, that will be determined in Subsection 3.3.2.

Figure 3.1: Three bubbles for varying radii ratio $\lambda$. The ratio for a Taylor bubble: $\lambda \geq 1.4$ as presented by Tomiyama et al.[1]. The red-dotted square describes the section that is plotted in Figure 3.2.

Table 3.1: Selected parameters from [1]

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Units</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>$\geq 1.4$</td>
<td>-</td>
<td>Tomiyama et al. [1]</td>
</tr>
<tr>
<td>$L_p$</td>
<td>1.0</td>
<td>m</td>
<td>Selected</td>
</tr>
<tr>
<td>$D_p$</td>
<td>24.8</td>
<td>mm</td>
<td>Tomiyama et al. [1]</td>
</tr>
<tr>
<td>$V_W$</td>
<td>1.0</td>
<td>$ms^{-1}$</td>
<td>Tomiyama et al. [1]</td>
</tr>
</tbody>
</table>
3.3 Numerical Setup

In this section the numerical setup for the purpose of this chapter is explained. This section consists of different parts, starting with Subsection 3.3.1 where the computational domain is presented. Then, Subsection 3.3.2 deals with the thermo-physical properties. The boundary conditions and the initial conditions are highlighted in Subsections 3.3.3 and 3.3.4, respectively. This is followed by Subsection 3.3.5 where the numerical schemes will be explained. This part of the chapter is finalized by Section 3.3.6, where the mesh and the time step \( \Delta t \) are presented.

3.3.1 Computational Domain

The computational domain consists of a vertical pipe with diameter, \( D_p \), and the length , \( L_p \). The length of the pipe is around 40 times larger than the diameter. The diameter and the length of the pipe are similar to the selected data set as shown in Table 3.1. The symmetry of the pipe is along the centerline, which is placed along the \( z \)-axis. Furthermore, because of the small dimensions the computational power required is relatively small. However, since the validation is done in two-dimensional setup an axi-symmetric wedge, a 'slice' of the cylinder, will be an appropriate selection for the physical domain. This will further reduce the computational effort. Figure 3.3 describes the axi-symmetric geometry of the wedge. Furthermore, the length of the pipe is placed along the \( z \)-axes and the radius along the radial direction. It should be noted that the axes in Figure 3.3 are Cartesian coordinates while the coordinates from the data set are cylindrical. The Cartesian coordinates are used since it is required for implementation in OpenFOAM. Figure 3.4 shows the computational domain for this case. Although, it is a two-dimensional geometry there is also a third axes in the \( y \)-direction. This is because simulation are performed within the framework of OpenFOAM where all cases should be assigned as three-dimensional mesh. To counter this, it is common to assign the third dimension as one cell thick in OpenFOAM. Furthermore, the assigned dimension in \( y \)-direction are 100 times smaller than the radius of the pipe. Hence, the influence of third dimension is infinitely small. The strategy for meshing is explained in section 3.3.6.

3.3.2 Thermo-physical properties and turbulence model

This section consists of two parts. Firstly, the thermo-physical properties will be introduced. Secondly, the turbulence model will be presented.

Thermo-physical properties

The fluid properties that are imposed in this case are listed in Table 3.2. These properties are implemented in the constant/transportProperties. This case contains two phases namely, water and air. The density and the kinematic viscosity for water are set to be \( 10^3 \) \([kgm^{-3}]\) and \( 10^{-6}[m^2s^{-1}]\), respectively. And, the density and the kinematic viscosity for water are
3.3 Numerical Setup

Figure 3.3: Schematic view of the wedge with the inlet, outlet, wedge front, wedge rear, axis of symmetry in Cartesian coordinates. Furthermore, $g$ and $V_w$ demonstrating the directions of the gravity and flow velocity, respectively.

Figure 3.4: The computational domain designed in OpenFOAM by implementing the dimensions from Table 3.1.

set to be $1.48 \cdot 10^{-5}$ [m$^2$s$^{-1}$] and 1.0 [kgm$^{-3}$], respectively. The surface tension coefficient between air and water is 0.07 [Nm$^{-1}$].

Turbulence modeling

The Reynolds number for this case is equal to 24800 that is obtained by applying the flow properties from Table 3.1 and 3.2 to (2.10). The characteristic length in this case is the pipes diameter $D_p$, $U = V_w$ and $\nu = \nu_w$. The flow is called turbulent when its Reynolds number is larger than the a commonly used limit of 4000. Accordingly, the flow in the current case is definitely turbulent and therefore a turbulence model is necessary to model the turbulence behavior. Subsequently, use is made of the standard $k - \varepsilon$ model with wall functions. The

\begin{table}[h]
\centering
\caption{Thermo-physical properties}
\label{tab:thermo_physical}
\begin{tabular}{|l|l|l|l|}
\hline
Properties & Symbols & Quantity & Units \\
\hline
Kinematic viscosity water & $\nu_W$ & $1.0 \cdot 10^{-6}$ & [m$^2$s$^{-1}$] \\
Density water & $\rho_W$ & $1.0 \cdot 10^4$ & [kgm$^{-3}$] \\
Kinematic viscosity air & $\nu_A$ & $1.48 \cdot 10^{-5}$ & [m$^2$s$^{-1}$] \\
Density air & $\rho_A$ & $1.0$ & [kgm$^{-3}$] \\
Surface tension & $\sigma$ & 0.07 & [Nm$^{-1}$] \\
\hline
\end{tabular}
\end{table}
initial values for the turbulent kinetic energy $k$, the dissipation rate $\varepsilon$ and eddy viscosity $\nu_t$ are determined by solving (2.41), (2.42) and (2.39) for $D = D_p$ and $U = \bar{V}_W$. All the quantities considering the turbulence modeling are added to Table 3.3.

<table>
<thead>
<tr>
<th>Table 3.3: Turbulence parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameters</td>
</tr>
<tr>
<td>Re</td>
</tr>
<tr>
<td>$\nu_t$</td>
</tr>
<tr>
<td>$k$</td>
</tr>
<tr>
<td>$\varepsilon$</td>
</tr>
</tbody>
</table>

### 3.3.3 Boundary conditions

The boundary conditions for the purpose of this chapter are motivated in this part. Two kind of boundary conditions are studied namely, a fixed one and a periodic one. Tables 3.4 and 3.5 summarizes the corresponding conditions for both options, which are explained in this subsection.

**Fixed boundary conditions**

Referring to Tomiyama et al. [1], the mean flow velocity, $\bar{V}_W$, is $1.0 \ [ms^{-1}]$. For this condition there are two options. The first one is to impose the inlet velocity in axial direction to $\bar{V}_W = 1 \ [ms^{-1}]$. The velocity profile for this option is schematically demonstrated in Figure 3.5, with $V_{av} = \bar{V}_W$. The flow is entering the pipe from left and progresses downstream to the right. Near the entrance, the viscous effects are limited to a thin boundary layer at the walls. Hence, at that region the flow is uniform across the channel and its velocity profile is bulky. This changes as the flow continuous downstream, while the viscous effects rises gradually. The velocity is developing from bulky profile to a parabolic one. This process stops after (hydrodynamic) entrance region/ length ($L_e$) is reached. After some time the flow become fully developed flow where the velocity profile does not change anymore and it is entirely dominated by viscosity. The velocity profile is parabolic, which is known as Poiseuille flow. Furthermore, the boundary layer thickness does not grow anymore but it will reach an asymptotic line that is equal to radius of the pipe ($\delta = r_p$). However, physically it is impossible to have purely an uniform velocity profile over the whole pipe diameter, as shown at the entrance of Figure 3.5. At the wall the no-slip conditions are applied, hence the velocity at the wall should be zero. So, it is unknown how the velocity profile is actually developing. This makes the first option less logical to apply. On the other hand, the second option is to impose the inlet velocity with the Poiseuille flow. In order to start with laminar flow with a parabolic velocity profile and to let the flow develop fully in the turbulent flow regime. Subsequently, in option two there is no such a physical contradiction as in option one. Hence, it is decided to proceed with the second option. In the next sub-paragraphs the conditions for fixed BCs are justified explicitly.
3.3 Numerical Setup

**Inlet:** The velocity at the inlet is imposed to the Poiseuille flow condition. This is derived from Navier-Stokes equations in various literatures, a.o. [71],[17] and [72], in both coordinate systems Cartesian and cylindrical. According to literature, the relations for the parabolic velocity for the current case are illustrated in (3.6) and (3.7). Figure 3.6 demonstrates the evolution of normalized streamwise velocity profile across the pipe length about the pipe diameter. In the same figure the Hagan-Poiseuille profile from (3.6) is also plotted. This is done in order to verify if the velocity is rightly imposed. The velocity profile at 1% of the pipe length ($L_p$) is compared with the Hagan-Poiseuille profile. It can be concluded that the velocity is correctly imposed. The slight difference is because the velocity profile taken about 1% of the pipes length and not exactly at the entrance of the pipe. Along the pipe length as the flow develops its velocity profile evolves from parabolic to bulky profile. Referring to Figure 3.6, from 12% to 15% of the pipe length. the flow does not change a lot. So from 15% of the length the flow is fully developed as its velocity profile that does not change anymore.

\[
U_x(r) = U_{max} \left( 1 - \frac{r^2}{r_p^2} \right), \quad (3.6)
\]

\[
\bar{V}_W = \frac{1}{2} U_{max}. \quad (3.7)
\]

**walls:** The wall of the wedge is imposed to no slip condition, meaning that the flow velocity is zero at the wall. This happens due to friction between the two phase of flow (water/air).
and the wall where the medium molecules that are in direct contact with the wall sticks to the wall surface. Hence, the relative velocity between medium molecules and wall is zero. The no-slip condition is result of large velocity gradient within the boundary layer which is proportional to the wall shear stress as described by (3.8). Where $u$ is flow velocity parallel to pipe wall along the boundary and normal to $r$. From Figure 3.6, it is important to emphasize that it seems that the no-slip condition does not verified. However, Figure 3.6 is based on data from the cell center while the no-slip condition is imposed on the wall. From Figure 3.7, it can be seen that the between cell center at the wall and the wall there is some space. So, from Figure 3.6, the velocity decreases from the pipe centerline to the last cell center at the wall as it is predicted. The negative sign is included in (3.8) to compensate the negative sign of the velocity gradient $-\frac{\partial u}{\partial r}$ in order that $\tau_w > 0$.

$$\tau_w = -\mu \left[ \frac{\partial u}{\partial r} \right]_{r=|r_p|}. \tag{3.8}$$

**outlet:** The velocity at the outlet is specified to have zero gradient. This means that the normal gradient is zero, hence the velocity at the outlet is a constant.

**wedge walls:** The wedge walls (front and rear from Figure 3.3) are 2 dimensional and axi-symmetric.
3.3 Numerical Setup

**center line:** The axis of the wedge which goes through the z-axis has a symmetry line condition.

**Periodic boundary conditions**

This subsection is devoted to periodic (cyclic) boundary conditions, which consists of two parts. The first part deals with the boundary condition. While, the second part is about how the flow is driven when periodic boundary conditions are applied. For demonstration use is made of pressure field \( p_{\text{rgh}} \), which is the standard pressure field within the OpenFOAM based VOF solver. The term \( p_{\text{rgh}} \) stands for dynamic pressure or as it is called modified pressure in Rusche’s Ph.D thesis (p.155) [28], (3.9). It is the difference between the total pressure \( p \) and the hydrostatic pressure \( \rho g \cdot x \). It is convenient to use \( p_{\text{rgh}} \) as boundary condition instead of \( p \), because when one specifies its value to zero, \( p_{\text{rgh}} = 0 \), the hydrostatic pressure is automatically set to zero as well. Accordingly, it take care of both hydrostatic pressure and static pressure. The next two subparagraphs defines the conditions at the inlet, outlet and at the wall of the domain. The wedge front, rear and the center line are the same for both, periodic and fixed, boundary conditions.

\[
p_{\text{rgh}} = p - \rho g \cdot x. \tag{3.9}
\]

**Inlet/outlet:** The inlet and the outlet of the wedge are imposed to be cyclic. This condition enables the inlet and the outlet as if they are connected physically. This condition reduced the distance between inlet and outlet and so the computational cost.

**walls:** The wall is specified as fixed-flux-pressure, which is an alternative for zero gradient condition that is imposed in cases where only pressure is present. However, in case where body forces such as gravity and surface tension are present fixed-flux-pressure is used in order to adjust the condition accordingly.

The wedge front, rear and the center line axis are the same for both boundary conditions, periodic and fixed. Tables 3.4 and 3.6 summarize the fixed and the periodic boundary conditions for all parameters, respectively. The boundaries that are the same for both conditions are inserted in Table 3.6. The conditions are listed in OpenFOAM notions.

**Introducing momentum source term**

In case of the periodic boundary conditions, the flow is driven by pressure gradient. It is necessary to generate a mean velocity that is equal to \( \bar{V}_W = 1.0 \ [m/s] \). This velocity is introduced by adding a momentum source term. It is done by calculating that momentum source as such that the volume average velocity in the whole domain is set to have the desired mean velocity. The volume average of a quantity is presented by a.o. Ni et al. in [73]. Setting the phase function \( X_k = 1 \) and \( \Psi_k = u_k \), the volume average velocity in (3.10) will
be obtained. With $u_k$ being the velocity in phase $k$ and $V_o$ being the total volume as defined in (3.11).

$$\bar{U}_k = \frac{1}{V_o} \int_{V_o} u_k dV,$$

(3.10)

$$V_o = \sum_k V_k.$$  

(3.11)

On the other hand, instead of calculating the volume averaged velocity in the whole domain one may choose to work with the volume averaged velocity of a $k^{th}$ phase. This is done by replacing the term of total volume, $V_o$, by volume that is occupied by $k^{th}$ phase, $V_k$. Furthermore, the phase function has to be set to phase fraction, $X_k = \alpha_k$. This is also presented by Ni et al. as Equation (2) in [73] and in this chapter is illustrated by (3.12). That represents the weighted volume averaged velocity. With $V_k$ being the total volume of phase $k$, as formulated in (3.13). So, if $\alpha_k = \alpha_{air}$ than the result of (3.13) will be equal to the total volume of the bubble. However, the ratio between the total volume of the domain ($V_o$) and the total volume of the bubble ($V_k$) is 1.1%. This means that there is not much difference between (3.10) and (3.12). Hence, for the current case both strategies are valid to be implemented.

$$\bar{U}_k = \frac{1}{V_k} \int_{V_o} \alpha_k u_k dV,$$

(3.12)

$$V_k = \int_{V_o} \alpha_k dV.$$  

(3.13)

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Inlet</th>
<th>Outlet</th>
<th>Walls</th>
<th>Internal field value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U$</td>
<td>cyclic</td>
<td>cyclic</td>
<td>noSlip</td>
<td>$(0,0,0)$</td>
<td>$ms^{-1}$</td>
</tr>
<tr>
<td>$p_{gh}$</td>
<td>cyclic</td>
<td>cyclic</td>
<td>fixedFluxPressure</td>
<td>$(=internalField)$</td>
<td>$kgm^{-1}s^{-2}$</td>
</tr>
<tr>
<td>$\alpha_{water}$</td>
<td>inletOutlet</td>
<td>inletOutlet</td>
<td>zeroGradient</td>
<td>$(=internalField)$</td>
<td>-</td>
</tr>
<tr>
<td>$\nu_t$</td>
<td>cyclic</td>
<td>cyclic</td>
<td>nutkWallFunction</td>
<td>$(=internalField)$</td>
<td>$m^2s^{-1}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Inlet</th>
<th>Outlet</th>
<th>Walls</th>
<th>Internal field value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U$</td>
<td>cyclic</td>
<td>cyclic</td>
<td>noSlip</td>
<td>$(0,0,0)$</td>
<td>$ms^{-1}$</td>
</tr>
<tr>
<td>$p_{gh}$</td>
<td>cyclic</td>
<td>cyclic</td>
<td>fixedFluxPressure</td>
<td>$(=internalField)$</td>
<td>$kgm^{-1}s^{-2}$</td>
</tr>
<tr>
<td>$\alpha_{water}$</td>
<td>cyclic</td>
<td>cyclic</td>
<td>zeroGradient</td>
<td>$(=internalField)$</td>
<td>-</td>
</tr>
<tr>
<td>$\nu_t$</td>
<td>cyclic</td>
<td>cyclic</td>
<td>nutkWallFunction</td>
<td>$(=internalField)$</td>
<td>$m^2s^{-1}$</td>
</tr>
</tbody>
</table>
3.3 Numerical Setup

Table 3.6: Conditions for fixed and periodic boundary conditions

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Wedge wall front</th>
<th>Wedge wall rear</th>
<th>Symmetric axis</th>
</tr>
</thead>
<tbody>
<tr>
<td>$U, \alpha_{water}, \nu_t$ and $p_{rgh}$</td>
<td>wedge</td>
<td>wedge</td>
<td>symmetry</td>
</tr>
</tbody>
</table>

3.3.4 Initial Conditions

It is essential to study when in the time the bubble can be introduced in the pipe. Two options are examined namely, when the bubble is introduced at time $t_0 = t = 0$ [s] and when it is introduced at time $t_0 + 0.10$ [s]. In this subsection both options are motivated. Initially, the bubble is inserted as an ellipse which is common for modeling a Taylor bubble as mentioned in different studies, o.a. by Behafarid et. al [63]. The initial form of the ellipse is described by (3.14) in cylindrical coordinates.

$$
\frac{z^2}{(0.5l_b - L_e)^2} + \frac{r^2}{r_p^2} < 1. \tag{3.14}
$$

From (3.14), the ellipse is shifted by one entrance length, $L_e$, in the $z$-direction. This is the length that is reached when the flow becomes fully developed at approximately 10 times the diameter of the pipe ($\approx 10D_p$), [74]. Hence, the position of the initial bubble (ellipsoid) is set to be one entrance length from the inlet. With $D_p$ being 24.8 [mm], the turbulent entrance length for this case is around 20% of the pipes length from the inlet. This is more or less in agreement with the results from Figure 3.6 where the velocity profile does not change anymore around 15% of the pipes length. Hence, the bubble is shifted by entrance length of $L_e = 0.2$ [m] in the $z$-direction. Furthermore, $l_b$ denotes the length of the initial bubble from (A.9). The value of $l_b$ is determined to be 0.15 [m] as shown in Appendix A. Moreover, the bubble is initialized first at time $t_0$ and than at time $t_0 + 0.10$ [s]. This done to test the effect when the bubble is initialized before, at time $t_0$ [s], and after, at time $t_0 + 0.10$ [s], the flow become fully developed. The condition of the flow is checked by running the simulation for only water ($\alpha_{water}$) till the velocity profile does not change anymore. For this case for both boundary conditions, fixed and cyclic, the velocity profile did not change anymore after $t_0 + 0.10$ [s], similarly as it is demonstrated for entrance length in Figure 3.6. The effects of different initialization times on two different boundary conditions are discussed in Subsection 3.4.1.

3.3.5 Schemes

For a CFD calculation the differential schemes are of a crucial importance. The ones applied for the computation of this case are summed up in Table 3.7. Similarly to boundary conditions, the numerical schemes are also tabulated in OpenFOAM notions. The differential schemes are methods according to which the terms of the governing equations are numerically approximated. The current system is categorized as a convective-dominated partial differential equation problem. The time derivatives of this system, ddtSchemes, are approximated by the Backward Euler or Implicate Euler schemes. Although this scheme is unconditionally stable, it adds some inaccuracy such as a numerical diffusion to the system. Hence, one
could argue to use Crank-Nicolson, which is a second-order method. However, in this case use is made of a RANS model for turbulence behavior. This adds already inaccuracy in the process of modeling. So, actually it does not matter which time integration is applied as long as it gives a stable solution. Therefore, a relatively simple but robust and unconditionally stable scheme, Backward Euler, is applied for time integration. The Gaussian integration is implemented for the discretization that is based on interpolation of values from cell centers to face centers. The interpolations are performed linearly as denoted by the keyword linear. The principle of this interpolation is nicely formulated by H. Jasak in [19], page 81. The divSchemes dictionary contains the advection terms where the convection term and diffusion term of transport equation are included. The convective terms like $\nabla \cdot (Uk)$, where the velocity $U$ delivers the advective flux, uses the Gauss linearUpwind grad(U), Gauss vanLeer, $k = \alpha$, and Gauss interfaceCompression schemes. While diffusion terms like $\nabla \cdot (\nu (\nabla U)^T)$ uses the Gauss Upwind and Gauss linear. The Laplacian term of the diffusion term in the momentum equation is specified in sub-dictionary laplacianSchemes. The Gauss scheme is used for discretization through linear interpolation scheme (linear) for diffusion coefficient ($\nu$). The surface normal gradient scheme ($\nabla U$) for Laplacian term is specified to be uncorrected because the mesh is orthogonal, as explained in Subsection 3.3.6. The later is actually defined within the sub-dictionary snGradSchemes. This is required in order to evaluate a Laplacian term using Gaussian integration. The aforementioned interpolationSchemes are set to be default with the keyword linear. The last sub-dictionary wallDist is specified to method meshWave that calculates the distance to nearest patch for all cells and boundary.

Table 3.7: Discretization schemes

<table>
<thead>
<tr>
<th>Categories</th>
<th>Mathematical notation</th>
<th>Dictionary</th>
<th>Discretization schemes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time schemes</td>
<td>$\frac{\partial}{\partial t}$</td>
<td>ddtSchemes</td>
<td>Euler</td>
</tr>
<tr>
<td>Gradient schemes</td>
<td>$\nabla$</td>
<td>gradSchemes</td>
<td>Gauss linear</td>
</tr>
<tr>
<td>Divergence schemes</td>
<td>$\nabla \cdot$</td>
<td>divSchemes</td>
<td>Gauss linearUpwind grad(U)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gauss vanLeer</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gauss interfaceCompression</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gauss Upwind</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gauss linear</td>
</tr>
<tr>
<td>Laplacian schemes</td>
<td>$\nabla^2$</td>
<td>laplacianSchemes</td>
<td>Gauss linear uncorrected</td>
</tr>
<tr>
<td></td>
<td></td>
<td>interpolationSchemes</td>
<td>linear</td>
</tr>
<tr>
<td></td>
<td></td>
<td>snGradSchemes</td>
<td>uncorrected</td>
</tr>
<tr>
<td></td>
<td></td>
<td>wallDist</td>
<td>meshWave</td>
</tr>
</tbody>
</table>

3.3.6 Meshing and the time step

This subsection consists of two parts. In the first part the strategy how the meshes are set up and mesh numbering are addressed. The second part is about determination of the time step $\Delta t$ that is closely related to mesh.
3.3 Numerical Setup

Meshing

Table 3.8 shows the list of the meshes that are used. A mesh number corresponds to amount of cells in the radial direction of the wedge. It is specified by symbol $N_r$, where subscript $r$ stands for radial direction. Throughout this chapter, when it is referred to a mesh it will denoted by its $N_r$ number. The sequence of the mesh numbering is described by series shown in (3.15),

$$N_{ri} = 2N_{ri-2},$$  

(3.15)

with $i = 1, 2, \ldots, n$, $N_{r1}$ and $N_{r2}$ begin 4 and 6, respectively. The amount of cells in the axial direction of the pipe is included in the second column of Table 3.8. Equation (3.16) represents the amount of cells in the axial direction,

$$N_{xi} = \text{int}\left(\text{round}\left(\frac{N_{ri}L_p}{r_p}\right)\right),$$  

(3.16)

with $L_p$ and $r_p$ being the length and the radius of the pipe, respectively. Multiplication between $N_r$ and $N_x$ results to total amount of cells that are added in column three. In this chapter the name working mesh or intermediate mesh refers to $N_r = 24$. Figure 3.7 demonstrates the meshed cross section on the left and on the right a part of the axial length of the wedge for mesh $N_r = 24$. The finest mesh and coarse mesh are corresponding with mesh $N_r = 96$ and $N_r = 4$, respectively. Although this chapter is about two dimensional simulation, for implementation to OpenFOAM there is a third dimension needed. To tackle that, $N_y$ is defined as the third dimension and it is specified to one cell thick in OpenFOAM. Because $N_y$ does not change, it is excluded from Table 3.8.

<table>
<thead>
<tr>
<th>Mesh number $N_r$</th>
<th>Cells $N_x$</th>
<th>Total cells</th>
<th>Mesh name</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>161</td>
<td>644</td>
<td>Coarse mesh</td>
</tr>
<tr>
<td>6</td>
<td>242</td>
<td>1452</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>323</td>
<td>2584</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>484</td>
<td>5808</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>645</td>
<td>10320</td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>968</td>
<td>23232</td>
<td>Working mesh/ Intermediate mesh</td>
</tr>
<tr>
<td>32</td>
<td>1290</td>
<td>41280</td>
<td></td>
</tr>
<tr>
<td>48</td>
<td>1935</td>
<td>92880</td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>2581</td>
<td>165184</td>
<td></td>
</tr>
<tr>
<td>96</td>
<td>3871</td>
<td>371616</td>
<td>Finest mesh</td>
</tr>
</tbody>
</table>

Time step $\Delta t$

The choice of time step depends of the mesh size, therefore it is essential to know how the time step and mesh size are related in order to maintain the stability. Therefore, Courant-Friedrichs-Levy (CFL) condition is necessary to ensure the convergence of the calculations.
The definition of this condition is expressed in (3.17), which is a dimensionless quantity. This condition stands for that the distance traveled by any information through the mesh should be smaller than the cell size of the mesh. It should be noted that this condition is a necessary criteria, but not sufficient for stability.

\[
\frac{u \Delta t}{\Delta x} \leq CFL,
\]

(3.17)

with,

- CFL for multiphase flows is commonly selected between 0.20 and 0.5 as shown i.g. in [75] and [63]. Accordingly, for this case it is chosen that CFL = 0.50,
- \( u \) being the maximum speed that is present in the domain. In this case \( u = U_{\text{max}} = 2.0 \, [\text{m/s}] \), and
- \( \Delta x \) being the length interval. For current case, length interval is determined for the finest mesh, \( \Delta x = \frac{1}{351} \, [\text{m}] \).

Inserting all known parameters into (3.17) a \( \Delta t \) of \( 6.5 \cdot 10^{-5} \, [\text{s}] \) obtained. This value is based on the maximum CFL condition of 0.5 for the finest mesh, \( N_r = 96 \). The maximum time step \( \Delta t_{\text{max}} \) is chosen to be \( 2 \cdot 10^{-5} \, [\text{s}] \) that is less than the calculated \( \Delta t \). The time-step has a fixed value that satisfies the CFL criterion of 0.5, hence the adjustTimeStep is set to be off.

### 3.4 Results

This section presents the results based on numerical setup from previous section. Figure 3.8 demonstrates the simulation of Taylor bubble for six time frames and for the finest mesh. This section is divided in three parts. Firstly, two different initial conditions with two different
3.4 Results

![Figure 3.8: Representation of Taylor bubble simulation for mesh $N_r = 96$ and $C_o = 0.5$](image)

Figure 3.8: Representation of Taylor bubble simulation for mesh $N_r = 96$ and $C_o = 0.5$
boundary conditions are studied, as listed in Table 3.9. From this study the most appropriate boundary condition and initial condition will be selected in Subsection 3.4.1. Secondly, in Subsection 3.4.2 the transient behavior of the bubble is analyzed and the best time, at which a quasi steady-state takes place, will be selected. The results discussed in Subsections 3.4.1 and 3.4.2 are based on mesh number $N_r = 24$. Subsequently, in Subsection 3.4.3 a grid dependency study is presented.

<table>
<thead>
<tr>
<th>Bubble Initialization</th>
<th>Cyclic BC.</th>
<th>Fixed BC.</th>
</tr>
</thead>
<tbody>
<tr>
<td>at $t = 0$</td>
<td>Case 1</td>
<td>Case 3</td>
</tr>
<tr>
<td>at $t = 10$</td>
<td>Case 2</td>
<td>Case 4</td>
</tr>
</tbody>
</table>

### 3.4.1 Boundary and initial condition results

Two different initial conditions are imposed on two different boundary conditions as shown in Table 3.9. Figures 3.9-3.12 demonstrate the results from the simulations that are being compared with the analytical approach of Tomiyama et al. The comparisons are done at $t = 0.15$ seconds and at $t = 0.25$ for both boundary conditions. So Figures 3.9-3.12 corresponds to following four cases:

- **Case 1**: morphology comparison for cyclic boundary condition with bubble initialized at $t = 0.0$ [s];
- **Case 2**: morphology comparison for cyclic boundary condition with bubble initialized at $t = 0.10$ [s];
- **Case 3**: morphology comparison for fixed boundary condition with bubble initialized at $t = 0.0$ [s]; and
- **Case 4**: morphology comparison for fixed boundary condition with bubble initialized at $t = 0.10$ [s].

Based on results from Figures 3.9-3.12, one can conclude that all four cases agree with the analytical approach of Tomiyama et al. [1]. However, in case of cyclic boundary conditions the flow is driven by pressure gradient. Referring to (3.9), the term with gravitational force causes pressure difference between inlet and outlet of the pipe. After each cyclic run the pressure at the inlet is higher than the outlet. So, the gravitational force cause a pressure jump between the inlet and the outlet after each cyclic run. Subsequently, this leads to that the Taylor bubble breaks and calculation crashes. This numerically unstable situation makes that the cyclic boundary condition less appropriate to proceed with. However, it is not because of cyclic boundary condition it self but because of the limitation within the VOF solver of OpenFOAM. Concerning the fixed boundary condition, the Taylor bubble shape is kept relatively more preserved when the bubble is initialized at time $t = 0.1$ than when the bubble is initialized at time $t = 0$. So, in conclusion the most appropriate boundary condition is fixed boundary condition with bubble initialized at $t = 0.1$, Case number 4.
3.4 Results

3.4.2 Transient analysis

The goal of this section is to determine a quasi steady-state based on the analysis of the transient behavior of the Taylor bubble. Figure 3.13 demonstrates the interface morphology of the bubble for the time \( t = 0.1 \) [s], \( t = 0.3 \) [s] and \( t = 0.6 \) [s] in comparison with the analytical approach of Tomiyama et al. The blue line is the bubble at initial time \( t = 0.1 \) [s] that has an ellipsoid form. The black line demonstrates the morphology of the bubble at \( t = 0.6 \) [s]. Furthermore, on the left side of the figure an intrusion through the bubble takes place at the center line of the pipe. This is also confirmed by simulation for finest mesh in Figure 3.8 for time frames 0.20, 0.30 and 0.40 seconds. This phenomena will be discussed in the next paragraph. In Figure 3.13, the green line predicts relatively the best the analytical approach. Hence, at time around \( t = 0.3 \) [s] is the right direction to look for a quasi steady-state time. It should be noted that the plots in Figure 3.13 are shifted in z-direction in order to compare the interface conveniently. Figure 3.14 shows the behavior of Taylor bubble that is traveling through the pipe. Each colored structure represents the 1/10 frame starting from
Figure 3.13: Representation of the morphology of the interface of the Taylor bubble for the initial time $t = 0.1$, and further in time at $t = 0.3$ and $t = 0.6$. The simulation results are validated with analytical (-o-) approach of Tomiyama et al.

t = 0.1 [s], when the bubble is initialized, up to $t = 0.6$ [s]. The radial and axial axes being scaled with the pipe radius $r_p$. Unfortunately with time and distance, the intrusion within the bubble increases for mesh $N_r = 24$. However, for the finest mesh the intrusion vanishes from $t = 0.5$ [s], Figure 3.8. For mesh $N_r = 24$, the morphology of the bubble at $t = 0.6$ [s], somewhere at 75% at the pipe length, is already very unstable. Therefore, it is decided to not analyze the contour plots after $t = 0.6$ [s]. For the quasi steady-state the morphology between $t = 0.3$ and $t = 0.5$ seconds are analyzed. Within these time range the shape of the bubble is changing relatively less. Figure 3.15 shows the morphology of simulated Taylor bubble for a time range between $t = 0.3$ and $t = 0.5$ seconds in comparison with the analytical approach. The shape of the simulated bubble for $t = 0.3$ [s] is the furthest from the analytical model of Tomiyama et al. The shape of the bubble between $t = 0.45$ and $t = 0.5$ seconds does not change much in time. Hence, the morphology of the simulation reaches the quasi steady-state around $t = 0.45$ [s]. So, for mesh $N_r = 24$ the appropriate time where the simulation riches its quasi steady-state is at $t = 0.45$ [s].

Intrusion

The intrusion in the bubble make the structure unstable. However, for the purpose of this chapter it is not significant. This chapter validates the interface morphology of Taylor bubble by comparing that to analytical approach of Tomiyama et. al. However, it is recommended for further studies to examine the following three points that may cause the intrusion within the bubble:
3.4 Results

**Figure 3.14:** Representation of the transient behavior of the simulated Taylor bubble for each 1/10 time frame starting from initial time $t = 0.1$ up to $t = 0.6$ seconds.

**Figure 3.15:** Morphology of the Taylor bubble for a range of time steps where quasi steady-state takes place in comparison with analytical (-o-) approach of Tomiyama et al. for mesh $N_r = 24$ with radial and axial axes scaled with the pipe radius $r_p$.
1. The influence of the 2 dimensional axi-symmetric wedge geometry on the bubble. It can be tested by performing the simulation for the same setting and conditions but in a 3D mesh, e.g. quarter of the pipe geometry.

2. The influence of the turbulence model. It can be tested by performing the simulation without any turbulence model included.

3. The influence of the shape of the initial bubble that has an ellipsoid shape. It can be tested by initializing the actual shape of Taylor bubble instead of an ellipsoid shaped bubble.

### 3.4.3 Grid-independence analysis

The goal of grid dependency study is to point out whether the calculations convergence when the mesh gets finer. The simulation is performed and post-processed for all meshes from Table 3.8 for:

- a fixed boundary condition with;
- the bubble being initialized at $t = 0.1$ [s]; and
- the quasi steady-state at time $t = 0.45$ [s].

Figure 3.16 illustrates a selection of the contour plots, namely for meshes $N_r = 4, 32, 48, 64$ and 96 in comparison with analytical approach of Tomiyama et al. [1]. As the mesh gets finer the grid convergences gradually to almost the exact shape as the analytical approach. Hence, the grid- independence is achieved.
3.5 Summary and conclusion

In this chapter the validation of morphology of Taylor bubble is performed using VOF-based solver of OpenFOAM. The results are compared with analytical model of Tomiyama et al. [1]. Equation (3.2) describes the analytical shape of the interface of the Taylor bubble. In order to reduce the computational effort, the domain is set to a 2D wedge with pipe’s radius and length being 12.4 millimeters and 1.0 meter, respectively. The simulation is tested for both fixed and cyclic boundary conditions. Taylor bubble is initialized as ellipse and has been introduced after the flow became fully developed. The dimensions of the bubble are determined by making use of the diameter ratio $\lambda$ from (3.1). Its value of at least 1.4 or bigger is specified for Taylor bubble as presented by Tomiyama et al. [1]. The calculations are performed for a time step of $2 \cdot 10^{-5}$ seconds. That time step is determined for a CFL number of 0.5 for the finest mesh that is available in the current case.

Based on results, the questions asked in the introduction of this chapter are answered as follows:

- the VOF based solver in combination with standard $k-\varepsilon$ model is able to predict the morphology of Taylor bubble. It has been shown that the shape of Taylor bubble agrees with the reference data. However, it is also observed that the bubble disintegrates after some time. Furthermore, the simulations are most stable for a fixed boundary

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.16.png}
\caption{Morphology of the Taylor bubble for different meshes in comparison with analytical approach of Tomiyama et al. for fixed boundary condition where the bubble is initialized at $t = 0.1$ second and for the quasi steady-state at time $t = 0.45$ seconds. With radial en axial axises scaled with the pipe radius $r_p$.}
\end{figure}
condition with bubble initialized at time 0.1 seconds. The quasi-steady state behavior of the bubble is determined to be at time $t = 0.45$ [s].

- although both boundary conditions agree with the results from the reference data, the fixed boundary condition is selected to proceed with. The simulation is numerically less stable in case of cyclic boundary condition. This is not because of the boundary condition itself but the limitation of the solver as explained in section 3.4.1.

- subsequently, a grid convergence study has been performed where it is shown that calculation converges as the mesh gets finer. Referring to Figure 3.16, it can be concluded that for a further research, e.g. 3D simulations, it is sufficient to use mesh $N_r = 32$.

Concerning the solver, it is recommended to adjust the capability of interFOAM in order to be able to perform simulation with cyclic boundary conditions. Although, the aim of this chapter is to validate the morphology of the Taylor bubble, which is done successfully, it is desirable to study the shape sensitivity of the bubble. Therefore, it is recommended to study the simulation in 3D mesh, to initialize the actual Taylor bubble instead of an ellipse and to study a different turbulence model against the current one.

Next chapter is about bubble shape sensitivity analysis.
Chapter 4

Bubble shape sensitivity analysis

4.1 Introduction

This chapter deals with last two items of Part 1 of the research objective as pointed out in Section 1.2. The objective of this chapter is to study the sensitivity of the Taylor bubble shape by altering three parameters. In particular, to inspect how the simulation is influenced by remodeling the initial bubble shape, by changing the turbulence model and performing the computation in a 3D mesh. These changes are applied through editing the computational setup from Chapter 3. This chapter is structured as following. The simulation strategies for the purpose of this chapter is explained in Section 4.2. Subsequently, the results are presented in Section 4.3. This chapter is finalized with the conclusion in Section 4.4.

4.2 Models and simulation

Referring to Figure 3.8, after some time the water intrudes the bubble from the back. This occurs because the velocity of water is relatively higher on the centerline of the pipe at a certain time. Therefore, it is important to understand how phenomena like intrusion influences the shape of the bubble. Or in other words how sensitive is the shape of the bubble due to remodeling the computational setup from previous chapter. Therefore, the cases in Table 4.1 are tested. Accordingly, this section is divided in a chronological order. In Subsection 4.2.1 the ellipse is replaced by an Actual Taylor Bubble for case ATB. This is followed by Subsection 4.2.2 where the standard $k - \varepsilon$ model is changed to a case where the turbulence behaviors of the flow are not modeled. This is called a no-model case, NM. For cases 3Dsym and 3Dcyc the simulations are performed in a 3D mesh with the symmetrical and cyclic conditions are imposed on the side planes, respectively. Therefore, a quarter pipe domain is used that is introduced in Section 4.2.3. The aforementioned cases are compared with case $N_r = 24$, which is described in Chapter 3.
### Table 4.1: Test cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Name</th>
<th>Sections</th>
</tr>
</thead>
<tbody>
<tr>
<td>ATB</td>
<td>Actual Taylor bubble initialized</td>
<td>4.2.1</td>
</tr>
<tr>
<td>NM</td>
<td>No Turbulence model is applied</td>
<td>4.2.2</td>
</tr>
<tr>
<td>3Dsym</td>
<td>Three Dimensional domain with symmetric side planes</td>
<td>4.2.3</td>
</tr>
<tr>
<td>3Dcyc</td>
<td>Three Dimensional domain with cyclic side planes</td>
<td>4.2.3</td>
</tr>
<tr>
<td>N&lt;sub&gt;r&lt;/sub&gt; = 24</td>
<td>The working mesh</td>
<td>3.3.6, Table 3.8</td>
</tr>
</tbody>
</table>

#### 4.2.1 Initializing the bubble as the actual Taylor bubble shape

Figure 4.1 demonstrates the cross section of the pipe for cases **ATB**, on the top, and **N<sub>r</sub> = 24**, at the bottom. The only difference between those cases is the shape of initialized bubble. The rest of the numerical setup is identical to Section 3.3.1. For a better view the wedge domain is mirrored about its centerline. For initialization of the bubble the shape is implemented and therefore the dimensions of the bubble need to be determined. Furthermore, for a fair comparison the volume of the bubbles in Figure 4.1 should be the same. The cross sectional area is determined with (4.1) that is in function of the analytical shape relation \( R(z) \) from (3.2). Note, that the parameters here are not normalized by \( r_p \). The volume of the bubble \( V_{ATB} \) is obtained by integrating (4.1) about the length of the bubble \( l_{ATB} \) as shown in (4.2).

\[
A_{ATB} = (R(z))^2 \pi, \tag{4.1}
\]

\[
V_{ATB} = \int_0^{l_{ATB}} A_{ATB} \, dz, \tag{4.2}
\]

- where \( l_{ATB} \) denotes the length of the bubble in meters for case of **ATB** in the initialized state.

As it is pointed out in Section A, the volume \( V_{ATB} \) should be equal to the hypothetical volume of the sphere from (A.2),

\[
V_{ATB} = V_s. \tag{4.3}
\]

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4.2 Models and simulation

The length of the bubble is obtained by solving (4.3) for \( l_{ATB} \). Accordingly, (4.3) is solved numerically since it has a term with fractional exponent. Firstly, (4.3) is rewritten in the form of,

\[
f(z) = \sum_i (R(\Delta z_i))^2 \Delta z_i - \frac{4}{3} \lambda^3 r_p^3,
\]

(4.4)

where \( \Delta z_i = \frac{L_p}{N} \) with \( L_p \) denoting length of the pipe and \( i = 1,2,3,...,N-1 \). For a range of \( z = [0, L_p] \), the root of (4.4) \( f(z) = 0 \) is solved while using the bisection method. The iteration convergence for a \( z = 0.63 \) [m], which is equal to the initial bubble length \( l_{ATB} \).

For verification the initial volume of case \( ATB \) is compared with case \( N_r = 24 \), as shown in Table 4.2. The discrepancy between the volumes is about 1.33%.

<table>
<thead>
<tr>
<th>Case</th>
<th>Bubble length at time ( t_i ) in [m]</th>
<th>( \alpha_{water} ) [-] at ( t_i + \Delta t ) [s]</th>
<th>discrepancy in %</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_r = 24 )</td>
<td>0.150</td>
<td>0.9089241133</td>
<td>-</td>
</tr>
<tr>
<td>ATB</td>
<td>0.126</td>
<td>0.9211970558</td>
<td>1.33</td>
</tr>
</tbody>
</table>

4.2.2 Turbulence model study

In case of \( N_r = 24 \), the standard \( k - \varepsilon \) model applied to model the turbulence behavior. The wall function models are specified through the turbulent viscosity \( \nu_t \). In case of \( NM \) the turbulence model is switched off entirely hence, the turbulent behavior is not modeled. It should be emphasized that this way of working tends to a Direct Numerical Simulation (DNS) and or Large Eddy Simulation (LES). However, it is certainly not the case in here. Since the current mesh is not fine enough to resolve all scales. So, the case is explicitly meant just to compare and to test the effect of the turbulence model by comparing case (\( NM \)) with \( N_r = 24 \). Besides the turbulence model the rest of the computation setup is identical to the case \( N_r = 24 \).

4.2.3 A quarter pipe 3D simulation

Figure 4.2 illustrates the 3D mesh for a quarter pipe domain with the dimensions as listed in Table 4.3. The reason why the calculations are done on a quarter pipe mesh is because it reduces the computing time. Contrary to the 2D mesh from Chapter 3 in this case the mesh is anisotropic. Basically, the mesh consists of two parts namely, the bulk part and the wall part. The mesh illustrated in Figure 4.2 has 8 cells in the bulk region with its length size is denoted as \( r_p - l_w \). At the wall region it has 9 cells with its length size being denoted as \( l_w \). Moving from the bulk towards the wall the cells are reducing in size gradually. The ratio between largest-smallest cell is \( \epsilon = 10 \). The mesh from Figure 4.2 is expressed as \( N_{rb} = 8 \), with number 8 describing the amount of cell in the bulk. The simulations will be performed for meshes \( N_{rb} = 3, 4, 6, 8, 12, 16 \) and 24. The cross section of the quarter pipe mesh is shown
on the left of Figure 4.2. As can be seen the cross section consists from a wall section, pair of side walls and a an axisymmetric centerline. The side walls are tested for both symmetrical conditions, case 3Dsym, and for cyclic conditions, 3Dcyc. In case of 3Dsym the flow is assumed to have a 2D planer flow field. This means that the tangential and radial velocity components are set to zero at the side wall planes. On the other hand, in case of 3Dcyc the flow field what leaves one of the side walls enters the other one. However, the quantities (i.e. velocity components) in the plane are not dominant comparing the axial quantities in this case. The boundary conditions in axial direction are the same as presented in Chapter 3. The

\[
\text{CFL condition is set to 0.2 that is a common for two-phase flow simulations. Accordingly, the initial time step is set to be } \Delta t = 1 \cdot 10^{-6} \text{ [s]. Referring to (3.17), in this case the } \Delta t \text{ is adjusted with varying } u \text{ in order to keep CFL constant. The 3D cases based on Large Eddy Simulation (LES). Therefore, the LES one-equation-eddy-viscosity (kEqn) sub-grid-scale (SGS) model is selected. This model is selected because of its simplicity to implement hence, convenient to use for a test. Similarly to strategy of previous two cases, in case of 3Dsym and 3Dcyc the goal is to just test the influence of the 3D calculation on the modeling of Taylor bubble. Hence, it should be noted, that no LES modeling procedure is performed so no } y^+ \text{ etc. are determined to generate the mesh. Figure 4.3 is a representation of the bubble that is initialized as an ellipsoid in a 3D quarter pipe domain. For the visualization the quarter pipe is mirrored as such to demonstrate a half pipe. Furthermore, the flow is fully developed at the entrance so, the entrance length is neglected.} 
\]
4.3 Results

In this section the results for the cases as listed in Table 4.1 are presented. The simulation for case ATB is analyzed by comparing with simulation for case $N_r = 24$ in Subsection 4.3.1. In Subsection 4.3.2 the result for case NM is demonstrated and compared with case $N_r = 24$. Finally, Subsection 4.3.3 is devoted for the results produced for the cases 3Dsym and 3Dcyc.

4.3.1 Actual Taylor bubble versus ellipse

Figure 4.4 shows, from top to bottom, the simulation results for cases ATB and $N_r = 24$, respectively. Both simulations are a representation at time $t_i + 0.35$ [s]. The simulation on top of Figure 4.4 demonstrates the simulation for the case where the bubble is initialized as actual Taylor bubble. While, the bottom one demonstrates the case where bubble is initialized as an ellipse. Comparing the simulations, it can observed that both shapes evolve to a similar Taylor bubble shape. Both bubbles have, slightly different, wake while evolving. The morphology of ATB is validated with analytical shape of Tomiyama et al. and compared with case $N_r = 24$ in Figure 4.9. The shape of ATB and $N_r = 24$ are almost identical and in agreement with the analytical model. Hence, changing the initialized shape of the bubble does not influence the simulation too much. In conclusion the bubble shows no sensitivity to changes of the initialized shape of the bubble.
4.3.2 Turbulence is modeled versus turbulence is not modeled

In previous chapter it is already demonstrated that when the bubble is rising through the liquid it creates wake at its tail and it develops a film around itself, which is also explained in Section 2.3.1. These two phenomena are related to the shape of the bubble that is area of interest in this chapter. Figure 4.5 shows the results of the simulations at $t_i + 0.35$ [s] for cases $N_r = 24$ and $NM$, respectively. The following observations are made:

- the air bubble in case of $NM$ is much longer and the overall diameter is smaller with a sharper bubble head;
- the air bubble in case of $NM$ start to dismantle earlier in time, but the process is less intense comparing to case $N_r = 24$; and
- the air bubble in case of $NM$ is far ahead in time comparing with case $N_r = 24$. This means that the turbulence model influences the bubble rise velocity significantly.

These observations are analyzed as follows. Generally, the introduction of the bubble into the flow increases the velocity gradient, $\frac{\partial u}{\partial r}$. The velocity gradient is linearly proportional to

1. wall shear stress from (3.8), and

2. the eddy viscosity from (4.5), where $l_{mix}$ denoting the mixing length. That is the distance that is traveled by a turbulent whirl before it vanishes due to mixing.

$$\nu_t = \left| \frac{\partial u}{\partial r} \right|^2 l_{mix}, \quad (4.5)$$

In other words, increment in velocity gradient due to introduction of the bubble leads to an increment in friction and turbulent eddy viscosity locally. Subsequently, due to high turbulent
viscosity locally the bubble dismantles intensively as can be seen in case of $N_r = 24$. In case of NM where no-model is used, the bubble experiences less resistance to rise. The morphology of case NM is validated with the analytical model of Tomiyama et. al and compared with case $N_r = 24$ in Figure 4.9. Qualitatively the shape of NM is in agreement with the analytical model and $N_r = 24$. However, the shape is not entirely the same as described by the analytical model. This is logical because the results for case NM are not realistic since the turbulence is not modeled. While, modeling turbulence behavior is necessary in this case. Based on these results, one may conclude that the turbulence model influences not only the bubble shape but also the bubble rise velocity significantly. Furthermore, Figure 4.6 manifests the results for cases ATB, where no turbulence model is used, and NM. The results from Figure 4.6 confirms the conclusion drawn in previous subsection that initialization of an actual Taylor bubble does not influences the shape of the bubble significantly.

Figure 4.5: From top to bottom, representation of the simulations for cases $N_r = 24$ and NM at plus $t_i + 0.35$ [s].

Figure 4.6: From top to bottom, representation of the simulations for cases ATB with no turbulence model applied and NM at $t_i + 0.35$ [s].
4.3.3 3D versus 2D simulation

The model for the current subsection is adapted accordingly to the findings made in subsections 4.3.1 and 4.3.2. Figures 4.7 and 4.8 represent the simulations for cases 3Dsym and 3Dcyc, respectively. The following observations are made:

- from Figure 4.7 to 4.8, the head of the bubble is similar for both cases. While, the tail of the bubble are different.
- in case of 3Dcyc, it is observed that the water pushes from the back to intrude the bubble. This means that at that time the velocity of the water is relatively higher at the centerline of the pipe.
- from Figures 4.7 and 4.8 it can be observed that grid convergence is achieved as the mesh gets finer, from top to bottom, the shape of the head of the bubble do not changes.

![Figure 4.7](image)

Figure 4.7: Representation of the simulation for case 3Dsym at $t_i + 0.35$ [s]. The simulations are demonstrated of meshes $N_{rb} = 3, 4, 6, 8, 12, 16$ and 24, from top to bottom.

Accordingly, in Figure 4.9, the morphology for 3Dsym and 3Dcyc are validated with the analytical model of Tomiyama et. al [1] and compared with 2D cases. Comparing 3Dsym to 3Dcyc, it can been seen the shape for both cases are almost identical. Carefully, one can suggest that the of 2D case NM is in agreement with 3D cases. Furthermore, the 3D cases are qualitatively in agreement with the analytical model and the 2D case, $N_r = 24$. However, the bubble head in case of 3D are relatively sharper than it is predicted by the analytical model. This is can be justified by the fact that there is no an adequate LES modeling procedure is
Figure 4.8: Representation of the simulation for case 3Dsym at $t_i + 0.35$ [s]. The simulations are demonstrated of meshes $N_{rb} = 3, 4, 6, 8, 12, 16$ and $24$, from top to bottom.

considered in those cases. Since the purpose of this chapter is only to examine how the three parameters, as mentioned in the introduction, influences the shape of the bubble.
4.4 Summary and Conclusion

In this chapter the sensitivity of the bubble shape is analyzed. The goal is to test how the bubble is influenced by testing the cases from Table 4.1. Based on the results the following conclusions are drawn:

- by observing the simulations from Figures 4.5 and 4.6 it can be concluded that by initializing an actual Taylor bubble instead of an ellipse does not change the end result of the simulation significantly. This observation is confirmed by comparing the the morphology for case ATB to analytical model of Tomiyama et al. [1] and case $N_r = 24$.

- by comparing the results for case NM with $N_r = 24$ in Figure 4.5, it can be concluded that the turbulence model influences not only the bubble shape but also the bubble rise velocity significantly. This is because the presences of the bubble increases the velocity gradient. This leads to an increment of the friction which, subsequently increases turbulent eddy viscosity locally. By testing the case NM, it is shown that the bubble experiences less resistance from the local viscosity. From Figure 4.9 it can be seen that the bubble’s head for NM is sharper than predicted by the analytical model. However, the shape of the bubble is, qualitatively, in agreement with analytical model and $N_r = 24$. So if one shifts the plot of NM from Figure 4.9 upwards it match the analytical model by shape.

- from Figures 4.7 and 4.8 it can be concluded that performing the calculations in a 3D
setting does influence the bubble shape. It is also shown that the bubble shape is affected whether a symmetric or cyclic condition is imposed to the side walls of the quarter pipe domain. The bubbles head are almost identical for cases 3Dsym and 3Dcyc, as shown in 4.9, but the tail region of the bubbles are different. Similarly to case NM, the shape of the bubbles are qualitatively in agreement with analytical model and case \( N_r = 24 \). While, the size of the bubble’s head does not match with the analytical model entirely.

So referring back to objective of this chapter, the bubble shape is sensitive to the turbulence model and the mesh but not so mush to a particular initialized shape of the bubble. The findings from this chapter have initiated a Taylor bubble LES study. That study is conducted as a separate project parallel to this project. The LES study is used as the reference data for 3D Taylor bubble morphology validation in the next chapter.
Chapter 5

3D Taylor bubble morphology validation

5.1 Introduction

This chapter is dedicated to Taylor bubble morphology validation against Large Eddy Simulations (LES) data set presented by Frederix et al. in [2]. The objective of this chapter is to model Taylor bubble regime in a vertical pipe while using the OpenFOAM-based VOF solver with the modified time integration scheme from Section 2.2.4. In addition, the turbulence behaviors should be modeled with a RANS method in which the turbulence is damped at the interracial area as addressed in Subsection 2.3.2. The latter one is the main focus point of this chapter. Based on the analysis from previous chapter, the high velocity gradients at the free surface (interface between air and water) generate high turbulence throughout the two phase flow when eddy viscosity models (EVMs) are used. Hence, a term is introduced into the RANS model equation in order to model a large scale interface [3], such as Taylor bubble. The simulations are performed on a fully 3D mesh. Moreover, the following questions should be answered at the end of this chapter:

- is the solver with modified time integration scheme in combination of a modified RANS model able to model Taylor bubble morphology properly?
- what is the appropriate damping term for the given conditions?
- to what extend the modification improves the simulation results in case where the turbulence behavior of the flow are model by a RANS?

The chapter’s sections are structured as follows. The LES test data set is described in Section 5.2. In Section 5.3 the numerical methodology is explained. The simulation strategy is addressed in Section 5.4 and that is followed by Section 5.5 where the results are presented. Based on the results a conclusion is drawn in Section 5.6.
5.2 Large eddy simulation dataset description

The study presented by Frederix et al. [2] is selected as a benchmark against which the validations will be done. In the first part of that study a rising Taylor bubble LES is performed in a vertical pipe with diameter $D = 50.8 \text{ mm}$ for a Reynolds number of $Re = 16 \cdot 10^3$. The work from [2] is carried out along the current chapter and it is initiated by the findings from Chapter 4. Generally, the idea of the LES is to compute a full unsteady Navier-Stokes calculations for motion scales of the order of the grid size or larger. Where both the mean flow and the large, energy-containing eddies are exactly computed. While the smaller sub-grid-scale motions are being modeled by a turbulence model. In Frederix et al. [2] a method is applied where no-model, implicit LES, is used for the SGS motions. The principles of that method are formulated by Komen et al. in [76]. The technical data from Frederix et al. [2] are shown in Table 5.1.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Symbols</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydraulic diameter</td>
<td>$D$</td>
<td>50.8</td>
<td>mm</td>
</tr>
<tr>
<td>Axial length of the pipe</td>
<td>$L$</td>
<td>30$D$</td>
<td>mm</td>
</tr>
<tr>
<td>Mean flow velocity</td>
<td>$U$</td>
<td>0.322</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>Diameter of the bubble (initialized)</td>
<td>$DTB$</td>
<td>92.5$D$</td>
<td>mm</td>
</tr>
<tr>
<td>Length of the bubble (initialized)</td>
<td>$LTB$</td>
<td>6$D$</td>
<td>mm</td>
</tr>
<tr>
<td>Surface tension</td>
<td>$\sigma$</td>
<td>0.001</td>
<td>N m$^{-1}$</td>
</tr>
</tbody>
</table>

5.3 Numerical Setup

This section is about the numerical models and methods that are used for the context of this chapter. It is divided in the following subsections. The computational domain is presented in Subsection 5.3.1. Subsection 5.3.2 deals with the turbulence models. The boundary and initial conditions are pointed out in Subsections 5.3.3, which is followed by Subsection 5.3.4 where the temporal and spatial discretization schemes are introduced. The mesh generation is presented in Subsection 5.3.5. The CFL number and the time step were addressed in Subsection 5.3.6.

5.3.1 Computational Domain

Figure 5.1 shows a schematic 2D illustration of the geometry. Similarly to the previous two chapters, the geometry is a vertical pipe. It contains water and the ensemble air - water is moving upwards (co-currant) in the direction of the mean flow velocity $U$. The gravity is moving downwards which is represented by $g$. The dimensions are adopted from the LES benchmark as presented in Table 5.1, which are explained in Subsection 5.3.5. Figure 5.2 represents the computational domain for this case.
5.3 Numerical Setup

**Figure 5.1:** Schematic illustration of the pipe geometry in 2D with the air bubble having a cylindrical shape in the initialized state. The ensemble moving upward in the direction are denoted by mean flow velocity $U$ while gravitational acceleration $g$ acts in downwards direction.

**Figure 5.2:** Representation of the computational domain.

5.3.2 Turbulence models

For the context of this chapter first an appropriate RANS model is selected. The models that are considered are standard $k - \varepsilon$, $k - \omega$ and $k - \omega$ SST. Three single phase cases are set up for each of these candidates to model turbulence behaviors. The single phase results are compared with LES test data. Accordingly, the most appropriate model is selected to proceed with. Furthermore, in the previous chapter it is observed that a high velocity gradient at the interface between the bubble and water results in high turbulence generation, in both phases. Hence, a turbulence damping is needed in the interfacial area to model such a flow correctly. This is done by introducing a source term to the to be selected RANS model. In that source term the modified Egorov damping term, as presented in Subsection 2.3.2, is included.

5.3.3 Boundary and initial conditions

In this subsection the boundary and initial conditions are introduced. The inlet and the outlet of the domain are imposed to a cyclic boundary conditions, in analogous manner as explained in Section 3.3.3. At the walls the noSlip condition is set for the mean velocity $U$, the zeroGradient condition for volume fraction $\alpha_{\text{water}}$, the fixedFluxPressure for pressure $p_{\text{ref}}$ and the associated WallFunctions for turbulence related parameters. Moreover, the initial condition for velocity is equal to mean flow velocity $U = 0.322$ [m/s] at time $t = 0$. The flow inside the domain is water, $\alpha_{\text{water}} = 1$, and the pressure is set to zero. The initial conditions for turbulent parameters are listed in Table 5.2. To this end, the value of the turbulence parameters are set to an order of magnitude that is common in industrial applications. Furthermore, the air bubble is initialized at time $t = 0$, as illustrated in Figure 5.1. The bubble has a cylindrical initial shape with a diameter $D_{TB} = 0.925D$ and length that is $L_{TB} = 6D$. Furthermore, the bubble is introduced at $L/(2D) - 3 < z/D < L/(2D) + 3$ of the pipe. This is done so that the cylindrical bubble have enough time to develop to a
Taylor bubble. Since the boundaries are imposed to cyclic conditions, no entrance length is taken into account as it was the case for fixed boundary conditions (Dirichlet) from Chapter 3. Moreover, since the turbulence damping method is used at the interface it is not necessary to initialize the bubble after time $t_i$, when the flow is fully developed.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu_t$</td>
<td>$1 \cdot 10^{-6}$</td>
<td>$m^2 s^{-1}$</td>
</tr>
<tr>
<td>$k$</td>
<td>$1 \cdot 10^{-3}$</td>
<td>$m^2 s^{-2}$</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>1</td>
<td>$m^2 s^{-3}$</td>
</tr>
<tr>
<td>$\omega$</td>
<td>$1 \cdot 10^{-3}$</td>
<td>$s^{-1}$</td>
</tr>
</tbody>
</table>

5.3.4 Schemes

The spatial discretization schemes for this case are similar to that in Table 3.7. For the temporal discretization schemes use is made of the second order time integration scheme SDIRK from Subsection 2.2.4 instead of backward Euler or implicit Euler schemes. The default time integration of the VOF-based solver is modified by implementing SDIRK as introduced in Subsection 2.2.4.

5.3.5 Meshing

To reduce the cost, the industry is interested in uniform meshes with wall function applied instead of refined mesh at the wall. For that reason two meshes are tested for this case. The **G-Mesh**, that is refined at the wall in which the whole flow can be simulated. And the **T-Mesh**, that is uniform mesh where the turbulence behavior of the flow is modeled. The next two paragraphs describes how these two meshes are generated.

**G-Mesh** It is important to take the boundary layer parameters into consideration during meshing in order to simulate the flow properly. In this case use is made of the so called $\left(\frac{1}{7}\right)^{th}$ power law formulation to determine those parameters. The relations (5.1)-(5.5) for this law are derived and presented in different publications, such as [17]. Accordingly, the parameters are determined and inserted in Table 5.3. Reynolds number in Table 5.3 is based on characteristic length $D$ from Table 5.1. Substituting the Reynolds number into (5.2) the friction coefficient $C_f$ is calculated. The wall shear stress $\tau_{wall}$ and friction velocity $U_\tau$ are obtained solving (5.2) and (5.3) for the known parameters. The wall spacing $\Delta s$ from (5.4) is determined for dimensionless wall distance of $y^+ = 1$. The dimensionless diameter is obtained by solving (5.5), which is used to generate the mesh. All the determined parameters are added in Table 5.3.

\[
C_f = \frac{0.026}{Re^{1/7}},
\]  

(5.1)
\[ \tau_{\text{wall}} = \frac{C_f \rho U_{Mao}^2}{2}, \] (5.2)

\[ U_\tau = \sqrt{\frac{\tau_{\text{wall}}}{\rho_{\text{water}}}}, \] (5.3)

\[ \Delta s = \frac{y^+ U_\tau}{\nu_t}, \] (5.4)

\[ D^+ = \frac{D}{\Delta s}. \] (5.5)

**Table 5.3:** Boundary layer parameters for the pipe geometry for \( y^+ = 1 \).

<table>
<thead>
<tr>
<th>Quantities</th>
<th>Parameters</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Re )</td>
<td>Reynolds number</td>
<td>16357.6</td>
<td>-</td>
</tr>
<tr>
<td>( C_f )</td>
<td>Friction coefficient</td>
<td>0.00650</td>
<td>-</td>
</tr>
<tr>
<td>( \tau_{\text{wall}} )</td>
<td>Wall shear stress</td>
<td>0.337</td>
<td>( kgm^{-1}s^2 )</td>
</tr>
<tr>
<td>( U_\tau )</td>
<td>Friction velocity</td>
<td>0.01836</td>
<td>( ms^{-1} )</td>
</tr>
<tr>
<td>( \Delta s )</td>
<td>Wall spacing</td>
<td>0.0545</td>
<td>( mm )</td>
</tr>
<tr>
<td>( D^+ )</td>
<td>Dimensionless diameter</td>
<td>932</td>
<td>-</td>
</tr>
</tbody>
</table>

Moreover, the mesh is described as follows. The size of a cell in the axial direction is given by (5.6), in the span wise direction by (5.7) and in radial direction by (5.8). The number \( N \) is a dimensionless parameter that specifies the cell size in axial direction in the bulk. The meshes are denoted by a letter \( G \) and a number \( N \). Figure 5.3 demonstrates the **G-Mesh** for \( N = 60 \).

\[ \delta_{\text{axial}} = N \Delta s, \] (5.6)

\[ \delta_{\text{span-wise}} = \frac{1}{2} N \Delta s, \] (5.7)

\[ \delta_{\text{radial}} = C \Delta s, \] (5.8)

with,

- \( C \): starting from the wall where \( C = 1 \) and developing to the center of the pipe with a growth factor of 1.07 till \( C = \frac{1}{2} \), and
5.3.6 Time step and CFL number

The CLF number is set to 0.40. The associate time step $\Delta t$ is determined using (3.17) for $U$ and $\Delta s$. The calculated time step is equal to $6.8 \cdot 10^{-5}$ [s]. Furthermore, the adjustTimeStep is switched on, which means that the $\Delta t$ will be adjusted in order to maintain the maximum CFL of 0.40.

5.4 Simulation strategy

For validation the LES benchmark is selected. However, before using that as reference data, first the LES results are validated. Furthermore, before the final simulations are ran an appropriate RANS model should be selected. Hence, a simulation strategy is necessary to keep things in perspective. The strategy is to conduct the simulation in the following chronological steps.

1. Validate LES results against one or more reference data. Therefore, the two following analytical models and one experimental data set are selected:

   (a) analytical model of Tomiyama et al. [1], as described in Chapter 3, where shape of the bubble is in function of Reynolds number;
(b) analytical model of Dumitrescu [11] where shape of the bubble is in function of Weber number and Froude number; and

(c) experimental data set of Mao et al. [12], where study is done on motion of Taylor bubbles in a vertical pipe for a similar diameter and Reynolds number as the LES study.

2. Select an adequate RANS model and mesh (G or T) by comparing the single phase simulations with LES results. The choice for single phase is motivated as follows. In an ideal situation, the computational domain for the purpose of current chapter can be divided into three sections:

(a) a section that consists of two phase flow by means of air bubble, interface and water film;

(b) a section that consists of two phase flow by means of air bubble’s tail and associate wake; and

(c) a section that consists of only water (so single phase) far from bubbles tail and its wake.

Essentially, the condition in the third section should be similar to that of single phase flow. Hence, single phase simulation are ran for standard $k - \varepsilon$ model, $k - \omega$, and SST $k - \omega$ models. Subsequently, the results are compared to LES data at the third section. Accordingly, the most adequate model is selected. Afterwards, in the selected model the modified Egorov term, as explained in Subsection 2.3.2, is introduced. From now on this damping term is expressed as a $\delta$, which denotes the length scale in meters from (2.47).

3. Run the simulations for the selected RANS model in combination with the turbulence damping term.

4. Validate the Taylor bubble morphology for different value of $\delta$ with the LES simulations.

5. Select an appropriate $\delta$ and perform the grid-independence analysis.

5.5 Results

In this section the simulation results are presented. This section is distributed in the following sequence. Firstly, the LES simulations are validated against the selected analytical models and experimental data set in Subsection 5.5.3. Secondly, the results from the single phase simulations for three different RANS models are compared with the LES results and the most adequate model is selected in Subsection 5.5.2. Thirdly, in Subsection 5.5.3 the results for different $\delta$ are compared with the LES benchmark. For an appropriate $\delta$ a grid-dependence analysis is conducted in Subsection 5.5.4. A bubble shape analysis with respect to different $\delta$ is performed in Subsection 5.5.5. Finally, the streamlines inside and outside the bubble are shown in Subsection 5.5.6.
5.5.1 LES validation against analytical models and experimental dataset

Figure 5.5 demonstrates morphology of Taylor bubble for the LES and the reference data. The centerline of the pipe lies along the horizontal axis and its radius along the vertical axis. The LES results are presented for three different mesh sizes, namely \textbf{G25}, \textbf{G30} and \textbf{G60}. It can be observed that the shape of the bubble for \textbf{G30} and \textbf{G25} matches nicely with the experimental data. The experimental data and the LES results lies between the two analytical models. This is expected since both analytical models make assumption. Tomiyama’s model is a function of Reynolds number while Dumitrescu’s model is a function of Webber’s and Froude’s number from (2.12) and (2.11), respectively. Supposedly, the difference between the analytical models and LES data is due to the fact that both models neglected some of the flow properties. Furthermore, the morphology for \textbf{G60} is in agreement with the reference data qualitatively but the bubble in this case is relatively sharper. This means that mesh \textbf{G60} is too coarse for the LES applications. Hence, the LES results for \textbf{G30} and \textbf{G25} will be used for validation of RANS model based simulation in the next subsection.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.5.png}
\caption{Validation of Taylor bubble morphology for LES results against analytical model of Tomiyama et al. [1] and Dumitrescu et al. [11], and experimental data of Mao et al. [12]. In this figure the centerline of the pipe lies along the horizontal axes and its radius along the vertical axes.}
\end{figure}

5.5.2 Single phase simulations

In this subsection the results for standard $k-\varepsilon$, $k-\omega$ and $k-\omega$ SST models for meshes \textbf{G60} and \textbf{T60} are demonstrated. The single phase simulations for all three models are compared with the LES data. Figures 5.6 and 5.7 represents the normalized turbulent kinetic energy $k/U_t^2$ with respect to $r/R$ for both cases \textbf{G60} and \textbf{T60}. The following observations are made:

- for different mesh the standard $k-\varepsilon$ model has different results. In case of \textbf{G60}, the $k-\varepsilon$ values are higher than the LES. In case of \textbf{T60} its value keeps increasing at the wall. This model is not accurate because for application of standard $k-\varepsilon$ model a $y^+ >> 1$ is required, which is not the case here;
- on the other hand the results for models $k-\omega$ and $k-\omega$ SST are rather accurate;
- in case of \textbf{T60}, the turbulent kinetic energy for the RANS models does not decline to zero at the wall. This means that at the wall scales are not resolved; and
5.5 Results

- in case of **T60**, moving towards the wall the graphs for the RANS models are not smooth. This is an indication that in case of **T60** the mesh is not sufficiently fine, hence does not capture all scales while in **G60** it is the case.

The Figures 5.8 and 5.9 demonstrate the normalized axial velocity $U_z/U$ profiles with respect to $r/R$ for **G60** and **T60**, respectively. Besides the LES simulations, the velocity profiles for different RANS models are also compared with two other works by Eggers et al. [77] and WU et al. [78] for $Re = 5300$ and $Re = 44000$, respectively. Reynolds number of the current case is $16 \cdot 10^3$, hence the velocity profile should be somewhere between the two reference profiles for both meshes. By observing the Figures 5.8 and 5.9, the following can be noted:

- the profile with lowest Reynolds number forms a upper limit for both meshes;

- the profile of $k-\omega$ and $k-\omega$ SST models lies for both meshes on top of each other and form the lower limit;

- the profile for LES is just between the two reference profiles as it was predicted;

- the profile for $k-\varepsilon$ model varies for different meshes; and

- in case of **T60**, the scales on the wall are not resolved. This can been seen from RANS based velocity profiles that stops at certain point (cell center of the wall cell). This is also observed from Figures 5.6 and 5.7, where $k$ does not go to zero at the wall.

Based on the aforementioned observations, this subsection can be concluded by selecting a proper mesh and a suitable RANS model. The standard $k-\varepsilon$ model is not an adequate candidate for this case. Furthermore, there is not too much difference between $k-\omega$ and $k-\omega$ SST. However, to overcome the deficiencies in $k-\omega$ model it is recommended by to use the later model [34]. Moreover, in case of **G**-mesh the scales are resolved at the wall while in case of **T**-mesh information is missing near the wall. Hence, the decision is made to perform the simulations for **G**-mesh with RANS $k-\omega$ SST model. Table 5.4 shows the list of the meshes.

<table>
<thead>
<tr>
<th>Table 5.4: <strong>G</strong>-mesh list</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
</tr>
<tr>
<td>-----</td>
</tr>
<tr>
<td>G25</td>
</tr>
<tr>
<td>G30</td>
</tr>
<tr>
<td>G40</td>
</tr>
<tr>
<td>G60</td>
</tr>
<tr>
<td>G80</td>
</tr>
<tr>
<td>G100</td>
</tr>
</tbody>
</table>
5.5.3 Simulations for different turbulence damping terms

Figure 5.10 demonstrates the validation of Taylor bubble morphology for different damping term $\delta$ against LES benchmark. The term $\delta$ is a quantification for turbulence damping term at the air-water interface. When $\delta = 1 \times 10^{-4}$ [m], the turbulence model is damped entirely. So whenever the bubble passes and $\delta$ term is activated it damps all the turbulent kinetic energy $k$ in the surrounding. The simulation become a LES or DNS kind of case. On the other hand high values of $\delta$ leads to no damping at all, hence a non-modified RANS model. With aforementioned information in mind, the results in this section are analyzed. The observations made from Figure 5.10 are:

- the length of the bubble in case of LES is relatively shorter. This is because the LES
5.5 Results

Figure 5.10: Validation of Taylor bubble morphology for different $\delta$ and $C80$ against LES simulation dataset. The centerline of pipe lies along the horizontal axis and its radius along the vertical axis.

Simulations are run for longer time period, roughly 200 throughputs, while the SST cases are run for only 10 throughputs. Hence, the bubble in case of LES disintegrate relatively more in time than in case of $k-\omega$ SST simulations;

- paying attention to the bubble’s head, for $\delta \leq 2 \times 10^{-4}[m]$ it matches the LES dataset;
- concerning the whole bubble, including the tail, for $\delta \leq 2 \times 10^{-4}[m]$ the shape is in agreement with the LES.

Based on these observations, one may conclude that the most optimal damping term for this case is $\delta = 2 \times 10^{-4}[m]$. This conclusion is supported by Figure 5.11 where normalized turbulent kinetic energy $k/U^2$ at the centerline is plotted against the normalized axial length $z/R$ for different damping terms $\delta$. The perturbation seen at $z/R = 10$ manifests where the head of the bubble is located and the spike of the graph at $z/R = -10$ is where the tail of the bubble is located. As can be observed perturbation starting from bubbles head and ending at the tail of the bubble where its wake is created. For $\delta \leq 2 \times 10^{-4}[m]$ the turbulent energy is nicely damped at the interface. One can argue that $\delta = 3 \times 10^{-4}[m]$ is also a potential candidate, however from Figure 5.10 the shape of the bubble for $\delta = 3 \times 10^{-4}[m]$ is less accurate compared to $\delta \leq 2 \times 10^{-4}[m]$. Furthermore, from Figure 5.11 for $\delta > 3 \times 10^{-4}[m]$ the friction on the interface of the bubble increases very rapidly. So it moves toward a situation with a non-modified RANS model. On the other hand for $\delta = 1 \times 10^{-4}$ [m], the turbulence model is damped entirely. So it moves towards LES kind of case in coarse mesh. Hence, $\delta = 2 \times 10^{-4}[m]$ is indeed the most appropriate length scale term to proceed with.

5.5.4 Grid-independence analysis

Figure 5.12 demonstrates in time averaged Taylor bubble shape for modified $k-\omega$ SST model with the damping term $\delta = 2 \times 10^{-4}[m]$ in comparison with LES cases. As already mentioned,
the difference in size of the bubbles is due to the simulation duration. The LES case is run for a longer time. Furthermore, it can be observed that the bubbles in case of RANS are smeared out. This is because the simulated bubble oscillates, which is due to low surface tension that is used in this case, Table 5.1. The surface tension is adopted from the test case, Frederix et al. [2]. In that study, it is chosen for a low surface tension to limit the spurious currents as reported by a.o. Strubelj et al. in [13]. Hence, the bubble disintegrates relatively more compared to the RANS simulation. Comparing the shape of the bubble with each other and with the LES, the results does not change for different mesh size. Hence, the grid-independence is achieved for this case.

5.5.5 Taylor bubble shape analysis for different $\delta$

Figure 5.13 represents the shape of Taylor bubble for a series of $\delta$ for G80. The bubble on top is for $\delta = 1 \times 10^{-4}[m]$ where the turbulence is damped too much. As $\delta$ increases the procedure of disintegration of the bubble increase with it. The bubble at the bottom is where the friction on the interface due to high turbulence is not damped at all. These results can be carefully compared with the results from Chapter 4. For example, the shape of the bubble for $\delta = 32 \times 10^{-4} [m]$ has similarities with the 2D case, i.e. $N_r = 24$, where standard $k-\varepsilon$ is used to model the turbulence behavior. So based on Figure 5.13 one can concluded that the $\delta$ does what it is meant for, namely damping the turbulence model at the interface.
5.5 Results

5.5.6 Streamlines

Figures 5.14 and 5.15 illustrate the streamlines inside and outside the bubble for a coarse mesh $G_{100}$ and a fine mesh $G_{60}$, respectively. The streamlines are based on relative velocity field. Inside the bubble, air is pressed in the direction of the head of the bubble. When the air approaches the head, a vorticity contour is created. Similar procedure can be observed at the tail side of the bubble. From this figure it can be concluded that inside the bubble two vorticity cell are present. Outside the bubble, the bubble pushes the water in the positive $z$-direction. Because of the resistance of the water vorticity is generated at the nose side of the bubble. The falling film is creating a recirculation region at the rear of the bubble, which is called bubbles wake region. Furthermore, all the vorticity contours above the centerline of the pipe are anti-clockwise except the contours on the tail side of the bubble. All the contours beneath the centerline the other way around. There is a discrepancy between two figure in the wake region of the bubble. This is because in case of $G_{100}$ the mesh is coarse. As can be seen when the mesh gets finer more details are captured. Furthermore, there are four convection locations inside the bubble where vorticity is observed. Two of which are on the head side and two on the tail side of the bubble. These convection locations are in symmetric about the centerline of the pipe. The velocities at the centerline and along the walls are opposite to each other.
Figure 5.12: From top to bottom, demonstration of the Taylor bubble shape being averaged in time for LES G25 and G30, and for SST G40, G60, G80 and G100 for damping term \( \delta = 2 \times 10^{-4}[m] \).
5.5 Results

Figure 5.13: Demonstration of the bubbles for **G80** for $\delta = [1, 2, 3, 4, 8, 16, 32] \cdot 10^{-4}[m]$, from top to bottom.
Figure 5.14: Representation of streamlines inside and outside the bubble for $\delta = 2 \times 10^{-4}$ [m] and $G_{100}$.

Figure 5.15: Representation of streamlines inside and outside the bubble for $\delta = 2 \times 10^{-4}$ [m] and $G_{60}$. 
5.6 Summary and conclusion

Taylor bubble regime in this chapter is modeled by using the VOF based solver with a modified time integration scheme. Moreover, the turbulence behaviors of this flow are modeled by a modified $k - \omega$ SST model. The modified model activates a term at the interface in order to damp the turbulence model. Based on the results, the questions that are asked in the introduction of this chapter are answered as follows.

- in Figure 5.10 the morphology of Taylor bubble is validated against the LES results. As can been seen the shape of the bubble are matching for a certain $\delta$. It should be taken into account that the bubble in LES simulations is shorter because it was ran for a longer time, hence it disintegrated relatively more;

- from Figures 5.10 and 5.11 it can be concluded that $\delta = 2 \times 10^{-4} \text{[m]}$ is the the most accurate choice. For this term, the turbulence model is damped nicely at the interface while in the rest of the flow the turbulence behavior is modeled properly by the SST model;

- to which extent the term damps out the high turbulence generation at the interface depends on the value of $\delta$. It can be observed from Figure 5.13 the bubble start to disintegrate at $\delta = 3 \times 10^{-4} \text{[m]}$. For $\delta = 32 \times 10^{-4} \text{[m]}$ the bubble has the similar characteristics as seen in case of 2D modeling in Chapter 3.

In conclusion the solver with higher order time integration and modified RANS model is able to model Taylor bubble morphology accurately for a damping term $\delta = 2 \times 10^{-4} \text{[m]}$.

Next chapter gives a summary and concluding remarks of this project.
Chapter 6

Summary and Conclusion

This master’s thesis presents CFD simulation data for turbulent Taylor bubble flow (air-water) in a vertical pipe for co-current flow. For these simulations use is made of OpenFOAM’s standard VOF solver in combination with a conventional RANS model to capture the turbulence of the flow on one hand. On the other hand, use is made of NRG’s Runge-Kutta (RK) VOF solver with a modified RANS model to model the turbulent flow while damping excessive eddy viscosity at the interface. Modeling such flows is complex, especially when the flow is turbulent. Many attempts have been made to model Taylor bubble turbulent flow using high resolution capabilities like LES. However, high resolution calculations like DNS and LES involve very fine meshes which increase the demand on computational resources. Such high resolution calculations are not feasible for industrial applications. On the other hand RANS modeling is a popular and relatively cheap approach within the industry to fulfill the need. Since very fine meshes are not required, hence demand on computational resources are limited. Such an economical model is very attractive for the industrial applications where low computational cost matters. In case of single phase flow, RANS methods predict the turbulent behavior sufficiently accurate. However, the RANS method fails to model the turbulence behavior of two-phase flows with large scale interfaces like stratified flows. Moreover, very little is known on how a RANS method is doing in the setting of Taylor bubbles flow. Therefore, in Part 1 of this project the simulations are ran while using the standard OpenFOAM-based VOF solver with the standard $k - \varepsilon$ RANS model. In Chapter 3 and 4, it is shown that the 2D simulation in the setting of Tomiyama et al. [1] matches the analytical data. However, while the head of the bubble matches well with the analytical data the tail disintegrates. The disintegration of the bubble is due to the over-prediction of turbulence behavior while using RANS modeling like standard $k - \varepsilon$. This issue is addressed a.o. by Egorov who developed a model which damps the high eddy viscosity at the interface. A source term was introduced to the turbulence dissipation equations of $k - \omega$ model, which damps the high value of the turbulence model at the interface. However, it is reported that Egorov’s model is grid dependent. Frederix et al. have extended the Egorov model in order to make it grid-independent and demonstrated this for a test case [4]. In Chapter 5 results are demonstrated for $k - \omega$ SST model with Frederix’s approach. For a damping term $\delta/D = 3.9 \times 10^{-3}$ the turbulence model
is damped at the interface while in the rest of the flow the turbulence behavior is modeled properly by $k - \omega$ SST model. Furthermore, it is shown that due to Frederix’s modification the model becomes more stable and robust through which a grid-independence is achieved.

Referring to the first question asked in the research objective: *is OpenFOAM’s standard VOF solver with a conventional RANS model able to model turbulent Taylor bubble flow?* Based on findings made in part 1 of this project, it can be concluded that OpenFOAM’s standard VOF solver with a conventional RANS model is able to model the shape of the Taylor bubble regime in two-dimensional uniform mesh (a wedge) partially. It fails to model the Taylor bubble flow properly. This is because of huge velocity gradients, huge shear, excessive eddy viscosity production, which leads the bubble disintegration. Furthermore, from the bubble shape sensitivity analysis, it can be concluded that the initial bubble shape does not influence the final bubble shape significantly while the turbulence model does.

Referring to the second question asked in the research objective: *is NRG’s Runge-Kutta (RK) VOF solver with the modified RANS able to model turbulent Taylor bubble flow?* Based of the results from part 2 of this project, it can be concluded that NRG’s RK-VOF solver with the modified $k - \omega$ SST method produces more reliable results compared to a non-modified RANS model. The excessive production of eddy viscosity, which cause that bubble disintegrated, is successfully damped out at the interface, in two-phase case, while in the rest of the flow, where it is predominantly single-phase, the turbulence behavior is modeled properly by a conventional RANS model. Hence, the NRG’s RK-VOF solver with Frederix’s modification of Egorovs model is a promising approach for modeling turbulent two-phase flows with large interfaces.

Next chapter is about the recommendations for further work regarding improvement of the method.
Chapter 7

Recommendations

Although it is shown that NRG’s Runge-Kutta VOF solver in combination with modified RANS model is able to simulate the flow regime accurately, there is room for improvements mainly how the length scale $\delta$ is selected. For example to express $\delta$ in terms of Reynolds number. So that for a turbulent two-phase flow (with large interface) a $\delta$ can be selected depending from its Reynolds number. Furthermore, the knowledge presented in this report can be used for follow up studies on CFD simulation of turbulent Taylor bubble flow. Besides nuclear reactor applications, the lessons learned in this project are applicable to other industrial applications with similar rheology, e.g. water cooling system.
Bibliography


Appendix A

Dimensions of the bubble

In this section the initial shape of the bubble is determined. The bubble is initialized as an ellipse as demonstrated in Figure A.1. The idea is that ellipse will evolve to a Taylor bubble. This is a common procedure for modeling a Taylor Bubble, as mentioned in [63] and [75]. The shape of the ellipse is represented by (A.1) in cylindrical coordinates.

\[
\frac{z^2}{a^2} + \frac{r^2}{b^2} = 1, \tag{A.1}
\]

where,

- \(a\): half of the major axis of the ellipse, hence half of the length of the bubble \(l_b\), and
- \(b\): half of the minor axis of the ellipse, hence half of the diameter of the pipe \(r_p\).

Radius is of the pipe \(r_p\) is known and the length of the bubble \(l_b\) is determined in this section. This is done as follows. The volume of the initial bubble should be equal to the volume of the hypothetical sphere, formulated by (A.2).

\[
V_s = \frac{4}{3} \pi r_s^3. \tag{A.2}
\]

The volume of the ellipsoid is determined by taking the integral of the area of its cross section about the length of the ellipse. The cross section of the ellipsoid is circular and its area is variable since it is changing with its length. Equations (A.3) and (A.4) shows the relation for the volume of the ellipsoid and its cross sectional area, respectively.

\[
V_e = \int_{-a}^{a} A_e \, dz, \tag{A.3}
\]

\[
A_e = \pi r^2(z), \tag{A.4}
\]

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From (A.1), expressing \( r \) in \( z \) for \( b = r_p \) results to (A.5).

\[
r = \sqrt{\left[1 - \frac{z^2}{b^2}\right] r_p^2}.
\]  
(A.5)

Substituting (A.4) and (A.5) into (A.3), (A.6) is produced.

\[
V_e = \int_{-a}^{a} \pi r_p^2 \left[1 - \frac{z^2}{a^2}\right] \, dz.
\]  
(A.6)

The volume of the ellipsoid is obtained by solving (A.6),

\[
V_e = \frac{4}{3} \pi r_p^2 a.
\]  
(A.7)

Now there are two equations and one unknown. Solving (A.8) for \( a \) with \( r_s \) being as expressed by (3.1).

\[
V_e = V_s,
\]
\[
\frac{4}{3} \pi r_p^2 a = \frac{4}{3} \pi (\lambda r_p)^3,
\]
\[
a = \lambda^3 r_p.
\]  
(A.8)

With \( a \) being halve the length of the major axis makes that \( l_b \) is,

\[
l_b = 2r_p \lambda^3.
\]  
(A.9)

To solve (A.9) the diameter ratio \( \lambda \) is needed. That is found by assuming that that the volume of the hypothetical sphere will occupy 10% of the total volume of the pipe. The volume of the pipe is determined through (A.10).

\[
V_p = \pi r_p^2 L_p.
\]  
(A.10)

Accordingly, solving \( 0.1 \cdot V_p = V_s \) for \( \lambda \), (A.11) is obtained. Inserting the values for \( L_p \) and \( r_p \) from Table 3.1 into (A.11) the value of \( \lambda \) is calculated to be 1.82. Subsequently, filling the result from (A.11) into (A.9) the length of the bubble is calculated to be \( l_b = 0.15 \) meters. Furthermore, the value of \( \lambda \geq 1.4 \) that agrees with the conditions from Tomiyama et al. [1].

All dimensions of the ellipsoid are known to be in order to be implemented. This is done in Section 3.3.4.

\[
\lambda = \sqrt[3]{\frac{3L_p}{4r_p}} 0.1.
\]  
(A.11)
Figure A.1: A sketch of the ellipse, representing the initial condition of the bubble (blue) in the pipe.