A Study of Taylor Bubbles in Vertical and Inclined Slug Flow using Multiphase CFD with Level Set

by

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Abstract

Slug flow commonly occurs in gas and oil systems. Current predictive methods are based on mechanistic models, which require the use of closure relations to complement the conservation equations to predict integral flow parameters such as liquid holdup (or void fraction) and pressure gradient. These closure relations are typically developed either empirically or from semi-empirical models assuming idealized geometry of the interface, thus they carry the highest uncertainties in the mechanistic models. In this work, sensitivity analysis has determined that Taylor bubble velocity in slug flow is one such closure relation which significantly affects the calculation of these parameters.

The main objective is to develop a unified higher-fidelity closure relation for Taylor bubble velocity. Here, we employ a novel approach to overcome the experimental limitations: validated 3D Computational Multiphase Fluid Dynamics (CMFD) with Interface Tracking Methods (ITMs) where the interface is tracked with a Level-Set method implemented in the commercial code TransAT®. In the literature, the Taylor bubble velocity is modeled based on two different contributions: (i) the drift velocity, i.e., the velocity of propagation of a Taylor bubble in stagnant liquid, and (ii) the liquid flow contribution. Here, we first analyze the dynamics of Taylor bubbles in stagnant liquid by generating a large numerical database that covers the most ample range of fluid properties and pipe inclination angles explored to date ($Eo \in [10, 700]$, $Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^{3}]$, and $\theta \in [0^\circ, 90^\circ]$). A unified Taylor bubble velocity correlation, proposed for use as a slug flow closure relation in the mechanistic model, is derived from that database. The new correlation predicts the numerical database with 8.6% absolute average relative error and a coefficient of determination $R^2 = 0.97$, and other available experimental data with 13.0% absolute average relative error and $R^2 = 0.84$. By comparison, the second best correlation reports absolute average relative errors of 120% and 37%, and $R^2 = 0.40$ and 0.17, respectively.

Furthermore, two key assumptions made in the CMFD simulations are justified with simulations and experiments: (i) the lubricating liquid film formed above the bubble as the pipe inclines with respect to the horizontal does not breakup, i.e., the gas phase never
touches the pipe wall and triple line is not formed; and (ii) the Taylor bubble length does not affect its dynamics in inclined pipes. To verify the robustness of the first assumption, the gravity-induced film drainage is analytically modeled and experimentally validated. From this model, a criterion to avoid film breakup is obtained, which holds in the simulations performed. The second assumption is validated with both experiments and simulations.

Finally, simulations of Taylor bubbles in upward and downward fluid flow in vertical and inclined pipes are performed, from where it is concluded that an improvement of the current velocity prediction models is needed. In particular, Taylor bubbles in vertical downward flow where the bubble becomes non-axisymmetric at high enough liquid flows are remarkably ill-predicted by current correlations.

Thesis Supervisor: Jacopo Buongiorno
Title: Professor of Nuclear Engineering and Science, MIT
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Being loyal to the grad schedule, I find myself in the wee hours of a weekday night finishing this manuscript. My officemates are currently fighting for my office spot from which I can observe the busy Albany Street crossing with the emblematic Massachusetts Avenue. However, the views are not the reason of the craving: my spot has the reputation of accelerating its dweller’s project and making him/her the next graduate student to finish the PhD. The reputation as a haven for the next student to overcome successfully this enriching, uncertain and rewarding experience which is grad school.
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Chapter 1

Introduction

1.1 Motivation

The scientific evidence regarding the contribution of human activities to climate change was overwhelming in the Fourth Assessment Report of the Intergovernmental Panel on Climate Change (IPCC) in 2007 (IPCC, 2007), and it has been confirmed again in the last report (IPCC, 2013). CO$_2$ is a major greenhouse gas that plays a significant role in global warming. Princeton Professors Robert Socolow and Stephen Pacala introduced the famous Stabilization Wedges concept, a simple framework for understanding both carbon emissions cuts needed to avoid dramatic climate change and the tools already available to do so. They consider the Carbon Capture and Storage (CCS) and Enhanced Oil Recovery (EOR) system a very important stabilization wedge (Pacala and Socolow, 2004; Socolow and Pacala, 2006), that will facilitate a smooth transition from the current fossil fuel-based economy to another one based on clean energy free of carbon emissions. In CCS and EOR schemes (including their transport and separation systems), multiphase mixtures of oil, natural gas, water and CO$_2$ are piped between reservoirs and surface processing facilities. There, CO$_2$ emitted from large sources such as fossil fuel power plants, is captured at the source, transported to a stor-
age site and injected in secure geological formations deep underground (Deutch and Moniz, 2007). These formations include oil and gas fields, as well as natural underground reservoirs. Coupled with EOR, CCS' economic attractiveness is increased: CO₂ injection aids oil and gas recovery from depleted reservoirs, as it displaces hydrocarbons from the reservoir rock. In their study, Deutch and Moniz (2007) reported that CCS technology could prevent about 90% of the fossil carbon from reaching the atmosphere. Accurate prediction of slug flow, a very common multiphase flow regime present in these systems, in the injection and extraction pipes will improve calculation of the equipment performance reducing uncertainty in the projects' planning, increasing efficiency, and thus reducing costs and energy consumption.

Two-phase slug flow is a type of two-phase flow regime or pattern characterized by large bubbles named Taylor bubbles, separated by plugs of liquid called liquid slugs. The Taylor bubble is a bullet-shaped bubble that occupies a significant fraction of the pipe cross sectional area. The liquid slug separates two consecutive Taylor bubbles and carries smaller homogeneously distributed bubbles. The main flow regimes are shown in figure 1-1, where slug flow is depicted in figure 1-1c. For a given fluid, pressure and channel geometry, the occurrence of these flow regimes depend on the liquid and gas phase velocities. For example, figure 1-2 shows a typical flow regime map, in this case for an air-water mixture at 25°C and atmospheric pressure in vertical tubes of 5.0 cm diameter (Taitel et al., 1980). It can be seen that the flow regime depends on the combination of gas and liquid superficial velocities, \( v_{gs} \) and \( v_{LS} \), respectively. The superficial velocity is an artificial velocity calculated as if the given phase were the only one present in a given cross sectional area, thus defined as the phase volume flow rate over the cross sectional area.

The current simulation tools to predict multiphase flows are mainly two-fluid models, also called phenomenological or mechanistic models. They require additional equations, called closure relations, to complete the conservation equations of mass, momentum, and energy of each phase, so that flow parameters such as liquid holdup (void fraction) and pressure drop can be predicted. Slug flow mechanistic models represent the flow regime as a sequence of fundamental units, also called slug units. Each unit contains a Taylor
bubble and a liquid slug (figure 1-3). The unknown variables include the Taylor bubble velocity, $v_{TB}$, the Taylor bubble gas velocity, $v_{gTB}$, the Taylor bubble liquid velocity, $v_{LTB}$, the liquid slug gas velocity, $v_{gLS}$, the liquid slug liquid velocity, $v_{LLS}$, the Taylor bubble void fraction, $\alpha_{TB}$, the liquid slug void fraction, $\alpha_{LS}$, the Taylor bubble length, $L_{TB}$, the liquid slug length, $L_{LS}$, and the pressure drop in the Taylor bubble and liquid slug, $(dp/dL)_{TB}$ and $(dp/dL)_{LS}$, respectively. Mechanistic models differ from each other in the assumptions made to simplify the model, in the closure relations used to obtain a closed set of equations and in the flow regime transition models. The closure relations are typically developed either empirically (as fits to experimental data), or from semi-empirical models assuming idealized geometry of the interfaces, e.g. spherical or bullet-shaped bubbles, or spherical or
elliptical droplets. The physical reality of the situation is of course much more complex, as shown by any direct visualization of the two-phase flow regimes in pipes. Furthermore, the closure relations are often obtained from low pressure and small diameter pipes which makes the application to actual oil field conditions questionable. For example, the drift velocity of Taylor bubbles in inclined pipes of stagnant liquid is typically calculated based on the correlation of Bendiksen (1984), which was obtained with water as the liquid phase, whose properties differ significantly from the fluids of oil and gas systems. Given these limitations, it is clear why these closure relations carry the highest uncertainties in the mechanistic models. For example, the multiphase transient simulator OLGA® (Bendiksen et al., 1991), used by the great majority of the oil industry, may predict the pressure drop in a vertical riser with an error up to 80% (Belt et al., 2011).

In this work, it has been determined that the Taylor bubble velocity affects significantly the prediction of void fraction and pressure drop of these models (see chapter 3). Thus,
the main objective is to develop a higher-fidelity closure relation for Taylor bubble velocity in vertical and inclined pipes. Furthermore, we employ here a completely novel approach to overcome the limitations of experiments, the tool with which closure relations have been obtained hitherto: 3D Computational Multiphase Fluid Dynamics (CMFD) with Interface Tracking Methods (ITMs). CMFD is a promising tool in which the 3D conservation equations are solved on a relatively fine mesh, thus providing a more complete representation of the velocity, pressure and temperature fields. In the presence of turbulence, if all spatial and temporal scales are resolved, the approach is known as Direct Numerical Simulation (DNS); if only the large eddies are resolved and the smaller eddies are modeled, then the approach is called Large Eddy Simulation (LES) (Lakehal, 2010). In the CMFD context it is also possible to track the moving interface between phases. These are the so-called ITMs, which offer further improved predictive capabilities for multiphase flow. These methods, whose advent appeared in the 80s with the single-fluid formalism (Kataoka, 1986), track the interface between phases and resolve property gradients near them, which in principle allows for accurate calculation of the mass, momentum and energy exchanges, avoiding the use of empirical correlations or idealized geometrical assumptions. In ITMs, mass, momentum
and energy conservations of the two phases are formulated locally, and material properties are updated locally based on a characteristic function referred to as the marker function, $C(x, y, z, t)$. To track the interface, a topology equation is solved for this function $C$, which can represent the minimum distance to the interface (level-set method, LS, our case), or the volume fraction of one phase (volume-of-fluid method, VOF). For example, density $\rho$ is calculated as

$$\rho = \rho_1 C + \rho_2 (1 - C).$$

(1.1)

where subscripts 1 and 2 indicate the phases. To track the interface, the following topology equation is solved for $C$

$$\frac{\partial C}{\partial t} + u \nabla C = 0.$$

(1.2)

### 1.2 Thesis structure

This PhD Thesis contains eight chapters. Chapter 2 reviews the models used to predict the void fraction and the pressure drop in multiphase flow, going through its history. Chapter 3 comprises the sensitivity analysis performed to three of these slug flow mechanistic models (Orell and Rembrand, 1986; Ansari et al., 1994; Petalas and Aziz, 2000) in order to determine which are the dominant closure relations. The result is that the Taylor bubble velocity, $v_{TB}$, affects strongly both the void fraction and the pressure drop predictions. Thus, the thesis is focused on this correlation from there on. Chapter 4 includes a brief description and validation of the CMFD code used, the commercial software TransAT® (2014), is described and validated in chapter 4. The two key assumptions made in the CMFD simulations of Taylor bubbles are justified in chapter 5: (i) the lubricating liquid film formed above the bubble as the pipe inclines with respect to the horizontal does not breakup, i.e., the gas phase never touches the pipe wall and triple line is not formed; and (ii) the Taylor bubble length does not affect its dynamics in inclined pipes. To verify the robustness of the first assumption, the gravity-induced film drainage is analytically modeled and experimentally validated. From it a criterion to avoid film breakup is obtained, which holds in the simulations performed. The
second assumption is validated with both experiments and simulations. Once the numerical code and simulation assumptions are validated, we move to the modeling of Taylor bubble velocity. In the literature, the Taylor bubble velocity is modeled based on the correlation of Nicklin et al. (1962),

\[ v_{TB} = C_0 v_m + v_d, \]

where \( v_d \) is the drift velocity of the bubble in stagnant liquid, and \( C_0 v_m \) is the contribution of the mixture velocity, \( v_m \), which is the sum of the liquid and gas superficial velocities, \( v_m = v_{SL} + v_{SG} \), respectively. The first contribution, the bubble drift velocity, \( v_d \), is analyzed in chapter 6. There, the numerical database that we obtained for the most ample range of fluid properties and pipe inclination angles explored to date is described. Based on this database, a new drift velocity correlation that outperforms current models is proposed. Furthermore, other important flow characteristics, such as the length needed for the liquid to stabilize in front of the bubble, are analyzed. The second contribution of equation 1.3, that of the mixture velocity, \( v_m \), is analyzed in chapter 7. Based on the database properties and geometries of the previous chapter, a set of cases are generated including upward and downward flow. Similar hydrodynamic features as for the case of stagnant pipes are studied. Finally, the contributions of this work, conclusions and questions for future investigations are reported in chapter 8.
Chapter 2

Mechanistic Models Literature Review

2.1 Introduction

In this chapter, an introduction to the conservation equations used by the mechanistic models is presented through the 1D code OLGA (Bendiksen et al., 1991). Then, a brief history of the models used to predict the void fraction and the pressure drop in multiphase flow is given, including a literature review of the mechanistic models.

2.2 Mechanistic modeling: Equations

The mechanistic approach for the prediction of flow characteristics is based on physical criteria, as opposed to data fitting of the first empirical models (see Section 2.4.1). The 1D code OLGA (Bendiksen et al., 1991) is amply used by the oil industry. It accounts for three different fluid distributions: gas, the liquid bulk or film, and the liquid droplets. Thus, it uses three continuity equations, three momentum equations, and a mixture energy-conservation equation.
The conservation of mass for the gas phase is

\[
\frac{\partial}{\partial t}(V_g \rho_g) = -\frac{1}{A} \frac{\partial}{\partial z} (AV_g \rho_g v_g) + \psi_g + G_g, \tag{2.1}
\]

for the continuous liquid phase,

\[
\frac{\partial}{\partial t}(V_L \rho_L) = -\frac{1}{A} \frac{\partial}{\partial z} (AV_L \rho_L v_L) - \psi_g \frac{V_L}{V_L + V_D} - \psi_e + \psi_d + G_L, \tag{2.2}
\]

and for liquid droplets

\[
\frac{\partial}{\partial t}(V_D \rho_L) = -\frac{1}{A} \frac{\partial}{\partial z} (AV_D \rho_L v_D) - \psi_g \frac{V_D}{V_L + V_D} + \psi_e - \psi_d + G_D, \tag{2.3}
\]

where the subscripts \(g\), \(L\), and \(D\) indicate gas, liquid, and droplet phases, respectively, \(V\) is the volume fraction, \(\rho\) is the density, \(v\) is the velocity, \(p\) is the pressure, \(A\) is the pipe cross-sectional area, \(\psi_g\) is the mass-transfer rate per unit volume between the liquid and gas phases, \(\psi_e\) and \(\psi_d\) are the entrainment and deposition mass rates per unit volume, respectively, and finally \(G\) is the potential mass source rate per unit volume.

Secondly, the momentum conservation equations of the gas and liquid droplets fields are combined to yield a combined momentum equation where the gas/droplet drag term \(F_D\) is canceled out,

\[
\frac{\partial}{\partial t}(V_g \rho_g v_g + V_D \rho_D v_D) = -(V_g + V_D) \left( \frac{\partial p}{\partial z} \right) - \frac{1}{A} \frac{\partial}{\partial z} (AV_g \rho_g v_g^2 + AV_D \rho_D v_D^2) - \lambda_g \frac{1}{2} \rho_g |v_g| v_g \cdot \frac{S_g}{4A} - \lambda_i \frac{1}{2} \rho_g |v_r| v_r \cdot \frac{S_i}{4A} + (V_g \rho_g + V_D \rho_D) g \cos(\gamma) + \psi_g \frac{V_L}{V_L + V_D} v_a + \psi_e v_i - \psi_d v_D, \tag{2.4}
\]

whereas the equation for the liquid film is

\[
\frac{\partial}{\partial t} (V_L \rho_L v_L) = -V_L \left( \frac{\partial p}{\partial z} \right) - \frac{1}{A} \frac{\partial}{\partial z} (AV_L \rho_L v_L^2) - \lambda_L \frac{1}{2} \rho_L |v_L| v_L \cdot \frac{S_L}{4A} + \lambda_i \frac{1}{2} \rho_g |v_r| v_r \cdot \frac{S_i}{4A} + V_L \rho_L g \cos(\gamma) - \psi_g \frac{V_L}{V_L + V_D} v_a - \psi_e v_i + \psi_d v_D - V_L d (\rho_L - \rho_g) g \frac{\partial V_L}{\partial z} \sin(\gamma), \tag{2.5}
\]
where the subscript \( i \) refers to the interface, \( \gamma \) is the pipe inclination with respect to the vertical, \( \lambda \) is the friction coefficient, \( S \) is the wetted perimeter, \( v_r \) is the relative velocity defined by the slip equation

\[
v_g = R_D (v_L + v_r), \tag{2.6}
\]

where \( R_D \) is a distribution slip ratio, and \( v_a \) is a velocity that depends on other variables:

\[
\begin{align*}
    v_a &= v_L \text{ if } \psi_g > 0 \text{ and evaporation from the liquid film,} \quad (2.7a) \\
    v_a &= v_D \text{ if } \psi_g > 0 \text{ and evaporation from the liquid droplets,} \quad (2.7b) \\
    v_a &= v_g \text{ if } \psi_g < 0, \text{ which corresponds to condensation.} \quad (2.7c)
\end{align*}
\]

Finally, the model uses one single mixture energy-conservation equation,

\[
\frac{\partial}{\partial t} \left[ \rho_g V_g \left( E_g + \frac{1}{2} v_g^2 + gz \right) + \rho_L V_L \left( E_L + \frac{1}{2} v_L^2 + gz \right) + \rho_D V_D \left( E_D + \frac{1}{2} v_D^2 + gz \right) \right] = \\
- \frac{\partial}{\partial z} \left[ \rho_g V_g v_g \left( H_g + \frac{1}{2} v_g^2 + gz \right) + \rho_L V_L v_L \left( H_L + \frac{1}{2} v_L^2 + gz \right) + \rho_D V_D v_D \left( H_D + \frac{1}{2} v_D^2 + gz \right) \right] + H_S + U, \tag{2.8}
\]

where \( E \) is the specific internal energy, \( H \) is the specific enthalpy, \( H_S \) is the enthalpy generation rate from mass sources, \( U \) is the heat transfer rate from the pipe walls, and \( z \) is the elevation.

As it can be observed, there are more variables, 30, than equations, 9. The model is closed with the so-called closure relations. In this manner, the transfer of mass, momentum, and energy among the phases are calculated by these closure relations. Furthermore, other variables such as the velocity of Taylor bubbles or the void fraction in liquid slugs are also obtained by closure relations. In the following chapter, these expressions are analyzed in more detail for three particular mechanistic models.

Another characteristic of the mechanistic models is that the expressions used depend on the flow regime. The present model includes two flow regimes: the distributed regime, which contains bubble and slug flow, and the separated regime, which contains stratified and
annular-mist flow. Some terms of the previous conservation equations drop out depending on the regime; e.g., all the droplet terms vanish in the distributed flow regime. Also, the equations for the friction factors and wetted perimeters are affected by the regime.

2.3 Multiphase flow modeling: Properties

A multi-component mixture exhibits a region of multiphase equilibrium on a pressure and temperature diagram, unlike a single component fluid that shows only a one-dimensional saturation line describing the transition between phases. As pressures and temperatures change along the pipes, flashing of the volatile liquid phases (such as methane or CO₂) occurs continuously, so that mass transfer occurs between the gas and the liquid phases within the two-phase envelope. The mass transfer is typically calculated assuming equilibrium between the phases. A brief description of the two approaches used to simulate mass transfer for hydrocarbon systems (Campbell et al., 1984), the constant-composition or black-oil model, and the variable-composition or compositional model, is given here.

The constant-composition or black-oil model is the simpler one. The name, black-oil, refers to any liquid phase that contains dissolved gas, such as hydrocarbons produced from oil reservoirs. These oils, which are typically dark in color, undergo relatively small changes in composition within the two-phase equilibrium region. Therefore, an acceptable description of the fluid system is a constant-composition model. In this model, two parameters are needed to calculate the physical properties of the two phases: the dissolved gas/oil ratio, \( R_s \), which accounts for gas that dissolves (condenses) or evolves (boils) from solution in the oil, and the so-called oil formation volume factor, \( B_o \), which describes the shrinkage or expansion of oil phase caused mainly by changes of the dissolved gas. These two parameters can be measured in the laboratory or predicted with empirical correlations (for example, see Appendix B of Brill and Mukherjee (1999)). Two extra parameters are needed in the model if water is also present in the fluid: the dissolved gas/water ratio, \( R_{sw} \), and the water formation volume factor, \( B_{w} \).

On the other hand, for volatile oils and condensate fluids, vapor/liquid equilibrium (VLE)
is more accurate to describe mass transfer than the previous model parameters, as done in the compositional model. VLE calculates the vapor and liquid phases mole fraction and their composition in a fluid mixture using an iterative scheme to calculate equilibrium constants. First, the composition of each phase is obtained, and then their properties such as surface tension, density, viscosity, and enthalpy are calculated (for example, see Appendix C of Brill and Mukherjee (1999)). In general, VLE calculations are considered more accurate than black-oil-model parameters to describe mass transfer for oils and condensates with a gas/oil ratio (GOR) higher than 2,000 scf/STB. However, they are also more cumbersome to implement and computationally intensive.

2.4 Multiphase flow modeling: History

Early investigators treated multiphase flow as a homogeneous mixture of gas and liquid, using a nonslip condition and an assumption of thermal equilibrium between the phases which did not capture pressure drop correctly and overpredicted void fraction (Brill and Mukherjee, 1999). This approach is known as the Homogeneous Equilibrium Model (HEM).

Improvements to the homogeneous model considered slip (e.g. Hagedorn and Brown (1965)) and later also flow regimes (e.g. Duns and Ros (1963)). Furthermore, Zuber and Findlay (1965) and Wallis (1969) developed the so-called drift-flux model to calculate void fraction. This model employs a distribution parameter, $C_0$, and the drift velocity, $v_{gj}$, that are dependent on the flow regime, typically predicted by empirical flow-pattern maps. The distribution parameter, $C_0$, is calculated as

$$C_0 = \frac{\langle \alpha j \rangle}{\langle \alpha \rangle \langle j \rangle}, \quad (2.9)$$

where $\alpha$ is the void fraction, $j$ is the total volume flux, and $\langle \rangle$ indicates that the quantity is averaged over the channel cross section. In the drift-flux model the void fraction is related to the “drift-flux” or vapor velocity relative to the mixture velocity, thus implicitly accounting
for slippage between phases:
\[
\langle \alpha \rangle = \frac{\langle j_g \rangle}{C_0 \langle j \rangle + v_{gj}},
\]
(2.10)

where \( \langle j_g \rangle \) is the vapor volumetric flux. If \( v_{gj} = 0 \) and \( C_0 \approx 1 \), the drift-flux model reduces to homogeneous flow. If \( v_{gj} = 0 \), but \( C_0 < 1 \), drift-flux correlations yield the so-called 
\textit{algebraic slip equations}. Also, void concentration at the wall greater than at the center yields \( C_0 < 1 \), while the reverse condition is captured by \( C_0 > 1 \). There are a number of 

drift-flux correlations, where the difference among them is the characteristics of the drift flux 

parameters, \( C_0 \) and \( v_{gj} \). These correlations are used often in the nuclear industry.

In order to further improve the predictions, more complex models using a mechanistic 

approach based on physical criteria through the two-fluid formulation appeared (equations 

6.1 to 3.3b), the so-called \textit{phenomenological} or \textit{mechanistic models}. It was Taitel and Dukler 

(Taitel and Dukler, 1976) who first employed this concept to predict flow regime transitions. 

These models complete the set of conservation equations with \textit{closure relations}.

Herein, a brief literature review of the models used is presented. First, the models 

employed in the oil and gas industry are described, which can be classified into two categories: 

mixture models and mechanistic models. Then, a short review of the closure relations used 

by the nuclear industry is given.

\subsection{2.4.1 Oil and gas industry}

\textbf{Mixture models}

The mixture or empirical models can be classified into three categories (Brill and Mukherjee, 1999): (i) no slip, no flow pattern consideration (HEM), (ii) slip considered but no flow 

pattern, and (iii) slip and flow pattern considered. Tables 2.1 and 2.2 enlists these models, 

the flow regimes they cover, the pipe inclination applicability, the evaluated data, and the 

fluids, pipe geometry and flow conditions used for their development.

The first models, also known as HEM, did not take into account either slip or flow regime 
in their calculations. There, the gas and liquid phases are assumed to flow at the same
velocity. Only the correlation to calculate the friction factor is needed, without distinction for different flow patterns. Its predictions are only acceptable for situations in which the velocities of the two-phase are indeed close, e.g. dispersed bubbly. Examples of these models are Poettmann and Carpenter (1952), Baxendell and Thomas (1961), and Fancher and Brown (1963), being the latter two based on the method of Poettmann and Carpenter. Poettmann and Carpenter (1952) proposed a method to calculate the bottom-hole pressure knowing the surface data for oil wells, and the depth and pressure for gas-lift wells in vertical pipes. They used field data from 49 wells obtained from the Bureau of Mines, Bartlesville, Oklahoma, and the Phillips Petroleum Company. Baxendell and Thomas (1961) extended the work of Poettmann and Carpenter (1952) for high flow conditions in vertical pipes. To do that, the authors performed experiments directly in wells and compared their results with data shown in Poettmann and Carpenter (1952) and field data collected from two other fields. Fancher and Brown (1963) proposed a method to increase the applicability ranges of Poettmann and Carpenter (1952) to lower flow rates and density ranges. The authors performed experiments in a field well using oil, salt water and gas.

Located in between the first and second category we can find the model of Lockhart and Martinelli (1949): its pressure drop empirical correlation does not need the liquid holdup explicitly, but it implicitly accounts for slip between the phases. The authors used experimental data from other investigators for water, different types of oil, benzene and kerosene for the liquid phase, and air for the gas phase. They differentiated four types of two-phase flow depending upon whether each phase is flowing viscously or turbulently, and calculated the pressure drop through a non-dimensional parameter, $\chi$, equal to the square root of the ratio of the frictional pressure drop in the pipe if the liquid flowed alone to the pressure drop if the gas flowed alone. Furthermore, the parameter $\chi$ is a function of the fluid properties and pipe geometry.

In the second category of models, where the slip is considered but not the flow regime, a correlation is required for both the liquid holdup and friction factor. Herein, Hagedorn and Brown (1965) presented a model for a wide range of vertical two-phase flow conditions.
They employed a vertical experimental well of 460 m-long through three different pipe sizes, four different liquids (water and three oils) for the liquid phase and air for the gas phase, to develop correlations for flowing pressure gradient predictions of different tubing sizes, flow conditions and liquid properties. The authors also claimed that extrapolation to larger pipe sizes is possible to an engineering accuracy extent. The authors compared their model predictions with their experiment results and also data from Baxendell and Thomas (1961), Fancher and Brown (1963) and Gaither et al. (1963). Later, Eaton et al. (1967) proposed a model applicable for horizontal pipelines. The authors performed experiments using water, distillate and crude oil as the liquid phase, and natural gas as the gas phase. They developed a liquid-holdup correlation independent of the flow pattern, and postulated that a single energy-loss correlation would suffice for all flow regimes. They tested the model against their own laboratory data and also field data. Into this category also falls the model of Asheim (1986), where a linearized function for the liquid holdup was developed. The author did not perform experiments but tested his model with production-well data from the Forties and Ekofisk fields, and flowline data from Prudhoe Bay.

In the last category of models, both slip and flow regime are considered. First, the flow regime is determined, and then different liquid holdup and friction factor correlations are used depending on the flow pattern. Duns and Ros (1963) differentiated three regions depending on the gas throughputs: low (including bubble flow, plug flow, and part of the froth flow regime), intermediate (including slug and the remainder of the froth flow regime), and high (including mist flow) gas throughputs. They proposed six correlations, two for each region. Laboratory measurements were extended from the ones of Ros (1961), particularly the mist flow range of high gas flow rates. The test described by Ros (1961) consisted of a 10m-long measurement section and three diameters (d=3.20, 8.02, 14.23cm). Furthermore, air as the gas phase and water, mineral spirit, lubricating oil, and gas oil as the liquid phase were used. Orkiszewski (1967) considered four flow regimes (bubble, slug, transition and annular-mist flow regime) and modified the slug flow model of Griffith and Wallis (1961). The author tested the model with well data: 22 from Venezuelan heavy-oil wells and those from
Poettmann and Carpenter (1952), Fancher and Brown (1963), Baxendell and Thomas (1961) and Hagedorn and Brown (1965). Aziz et al. (1972) presented a model for vertical pressure drop prediction of single-phase liquid, bubble and slug flow regimes based on mechanistic considerations, similar to the modern mechanistic models. They tested the model against well data from Poettmann and Carpenter (1952), Orkiszewski (1967), Espanol et al. (1969) and the Energy Resources Conservation Board. Chierici et al. (1974) based their two-phase vertical flow model on that of Orkiszewski (1967), proposing a new model for the slug flow regimes avoiding empirical correlation coefficients. They tested their results against 31 oil wells and 6 gas wells. One year before the previous model, Beggs and Brill (1973) was the first to predict liquid holdup and pressure drop at all inclination angles, including downward flow. The correlations developed were based on two-phase flow of air and water in pipes of 27.4m long, and 2.54 and 3.81cm of diameter. For each pipe, liquid and gas rates were varied to observe all flow patterns when the pipes were horizontal: segregated, intermittent and distributed flow. They tested the model with their own experimental data. Later, Mukherjee and Brill (1985) presented a new unified model for bubble, slug, stratified and annular-mist flow regimes. They performed experiments for all inclination angles with kerosene and lube oil as the liquid phase and air as the gas phase at a pipe of 3.8cm diameter and 9.8m long. They tested the model against their experimental data and also field data from the Prudhoe Bay (Brill et al., 1981) and the North Sea (Rossland, 1981).

The best known multiphase flow codes using these models are the French TACITE (Pau- chon and Dhulesia, 1994), a drift-flux type model with one mass conservation equation for each phase, one mixture momentum equation, and one mixture energy equation, and TRAFLOW, which was developed by the Shell Oil Company.
## Table 2.1: Mixture or empirical models for multiphase flow

<table>
<thead>
<tr>
<th>Experiments Performed</th>
<th>Flow Regime Applicability</th>
<th>Inclination Applicability</th>
<th>Evaluated Data</th>
<th>Liquid Phase</th>
<th>Gas Phase</th>
<th>Inclination Angle</th>
<th>Pipe Diameter</th>
<th>Length</th>
<th>( P_h )</th>
<th>Flow Rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poettmann and Carpenter (1952)</td>
<td>-</td>
<td>Vertical</td>
<td>Bureau of Mines and Phillips Petroleum Company</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Baxendell and Thomas (1961)</td>
<td>-</td>
<td>Vertical</td>
<td>La Paz and Mara fields, Bureau of Mines and Phillips Petroleum Company, and in-house</td>
<td>Oil</td>
<td>Gas</td>
<td>90°</td>
<td>7.30, 8.89cm</td>
<td>1.829m</td>
<td>4,137–11,031kPa</td>
<td>( q_o = 3.2 \times 10^{-4} - 9.4 \times 10^{-3} \text{m}^3/\text{s} )</td>
</tr>
<tr>
<td>Panzer and Brown (1963)</td>
<td>-</td>
<td>Vertical</td>
<td>In-house</td>
<td>Oil, salt water</td>
<td>Gas</td>
<td>Vertical</td>
<td>6.03 cm</td>
<td>2,400m</td>
<td>23,000kPa</td>
<td>( q_L = 1.4 \times 10^{-4} - 1.2 \times 10^{-3} \text{m}^3/\text{s} ), gas-liquid ratios 18.7–1,680m(^3)/m(^3)</td>
</tr>
<tr>
<td>Lockhart and Martinelli (1949)</td>
<td>-</td>
<td>Vertical</td>
<td>In-house</td>
<td>Water, Oils, Benzene, Kerosene</td>
<td>Air</td>
<td>Vertical</td>
<td>0.149–2.58cm</td>
<td>0.67–15.24m</td>
<td>11–36kPa</td>
<td>n.a.</td>
</tr>
<tr>
<td>Hagedorn and Brown (1965)</td>
<td>-</td>
<td>Vertical</td>
<td>In-house and Baker (1958)</td>
<td>Water, three different oils</td>
<td>Air</td>
<td>Vertical</td>
<td>2.54, 3.175, 3.81cm</td>
<td>457m</td>
<td>n.a.</td>
<td>n.a.</td>
</tr>
<tr>
<td>Eaton et al. (1967)</td>
<td>-</td>
<td>Horizontal</td>
<td>In-house and Baker (1958)</td>
<td>Water, distillate, crude oil</td>
<td>Natural gas</td>
<td>Horizontal</td>
<td>5.08, 10.16, 43.2cm</td>
<td>520, 1,600m</td>
<td>( \approx 2,000–8,000\text{kPa} )</td>
<td>( q_o = 9.2 \times 10^{-5} - 1.0 \times 10^{-3} \text{m}^3/\text{s} ), gas-liquid ratios ( 0–23,000 \text{m}^3/\text{m}^3 )</td>
</tr>
<tr>
<td>Asheim (1986)</td>
<td>-</td>
<td>Vertical</td>
<td>Forties and Ekofsk fields; Prudhose Bay flowline data</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Duns and Ros (1963)</td>
<td>Low, intermediate, high gas throughputs</td>
<td>Vertical</td>
<td>In-house, Ros field</td>
<td>Water, mineral spirit, lubricating oil, and gas oil</td>
<td>Air</td>
<td>Vertical</td>
<td>3.20, 8.02, 14.23cm</td>
<td>10m</td>
<td>n.a.</td>
<td>( \nu_L = 0 - 3.2\text{m/s} ), ( \nu_g = 0 - 100\text{m/s} )</td>
</tr>
<tr>
<td>Orkiszewski (1967)</td>
<td>Bubble, slug, transition, annular-mist</td>
<td>Vertical</td>
<td>Venezuelan heavy-oil wells, and Poettmann and Carpenter (1952); Panzer and Brown (1963); Baxendell and Thomas (1961); Hagedorn and Brown (1965)</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
Table 2.2: Mixture or empirical models for multiphase flow (continuation)

<table>
<thead>
<tr>
<th>Flow Regime Applicability</th>
<th>Inclination Applicability</th>
<th>Evaluated Data</th>
<th>Experiments Performed</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Liquid Phase</td>
</tr>
<tr>
<td>Aziz et al. (1972)</td>
<td>Vertical</td>
<td>Poettmann and Carpenter (1952); Orkiszewski (1967); Españo et al. (1969) and Energy Resources Conservation Board</td>
<td>-</td>
</tr>
<tr>
<td>Chierici et al. (1974)</td>
<td>Vertical</td>
<td>Field data (oil and gas wells)</td>
<td>-</td>
</tr>
<tr>
<td>Beggs and Brill (1973)</td>
<td>Unified upward and downward</td>
<td>Water</td>
<td>Air</td>
</tr>
<tr>
<td>Makherjee and Brill (1985)</td>
<td>Unified upward and downward</td>
<td>Kerosene, lube oil</td>
<td>Air</td>
</tr>
</tbody>
</table>

$q_L = 0 - 1.9 \times 10^{-3} \text{ m}^3/\text{d}, q_g = 0 - 98 \text{ m}^3/\text{s}$
Mechanistic models

In 1976, Taitel and Dukler introduced a mechanistic approach for the horizontal flow regime predictions where the transitions were based on physical criteria (Taitel and Dukler, 1976). In these models, the flow regime is first identified and then pattern-specific closure relations are used to obtain the flow variables and, in last instance, the void fraction and pressure drop. The mechanistic models can be classified whether they are applied to one or more flow regimes. Furthermore, models can be differentiated by the applicable inclination angle (horizontal, slightly inclined, inclined, vertical and unified) within each category. Tables 2.3 and 2.4 enumerates different existing mechanistic models, including the flow regimes they cover, the pipe inclination applicability, the transition models, the evaluated data, and the fluids, pipe geometry and flow conditions used for their development. These models are briefly described here. Also, the mechanistic models of Orell and Rembrand (1986), Ansari et al. (1994) and Petalas and Aziz (2000) are studied in more detail in the following chapter.

First, we describe the mechanistic models for one flow regime. Fernandes et al. (1983) presented a hydrodynamic model for gas-liquid slug flow in vertical pipes based on “the physical processes thought to take place during slug flow”. The authors developed a set of 17 nonlinear algebraic equations in order to obtain the parameters of slug flow, such as the liquid slug void fraction and the pressure drop. The authors carried out experiments of turbulent slug flow air-water mixtures in vertical pipes, with which their model was tested. Later, Orell and Rembrand (1986) simplified the previous model and reduced it to 7 equations and 7 unknowns. The authors did not perform experiments, but compared their results with air-water experimental results from the literature (Brown et al., 1960; Brown and Govier, 1961; Griffith and Wallis, 1961; Akagawa and Sakaguchi, 1966; Subbotin et al., 1976; Fernandes, 1981). Andreussi et al. (1993) proposed a mechanistic model of slug flow in horizontal and near-horizontal pipes with new empirical closure relations. The authors performed experiments with air and water for several inclination angles: $\theta = 0^\circ, 0.3^\circ, \pm 3^\circ$. Later, Issa and Kempf (2003) proposed a transient slug flow model for the same inclination as before (horizontal and near-horizontal), where the flow field was allowed to develop naturally from any
given initial conditions as part of the transient calculation. The authors performed experiments with air and water. For vertical pipes, Oliemans et al. (1986) proposed a model for annular flow, where new correlations for interfacial friction and liquid fraction entrained were proposed. Several fluids were used in their experiments for both the liquid (water, ethanol, genklene) and the gas (air, steam) phases. The parameters of the correlations were obtained for small diameters, and the authors found that their extrapolation to large-diameter and/or high pressure systems was not completely satisfactory. Unified upward models for slug flow can also be found in the literature. Felizola and Shoham (1995) presented a unified model for slug flow in upward inclined pipes where new correlations for slug length and liquid holdup as a function of inclination angle are presented. They performed experiments with kerosene and air at inclination angles ranging from 0° to 90°. Later, Abdul-Majeed and Al-Mashat (2000) proposed a unified upward mechanistic model for slug flow. The authors compared the predictions of the liquid slug void fraction with data from Schmidt (1977) and Felizola (1992), and the pressure drop to the Tulsa University Fluid Flow Projects (TUFFP) well database that includes wells data from Poettmann and Carpenter (1952), Fancher and Brown (1963), Hagedorn and Brown (1965), Baxendell and Thomas (1961), Orkiszewski (1967), Chierici et al. (1974), Govier and Fogarasi (1975), Asheim (1986), various Master of Science theses from the University of Tulsa, and field data from several oil companies (Ansari et al., 1994).

Secondly, the so-called comprehensive multiphase flow models predict liquid holdup and pressure drop for several flow regimes, including transition criteria between them. In vertical pipes, Ansari et al. (1994) formulated a comprehensive model whose flow pattern prediction was based on Taitel et al. (1980), Barnea et al. (1982) and Barnea (1987). The flow behavior prediction consisted of different models for three flow regimes: bubble, slug, and annular. Later, Chokshi et al. (1996) proposed a mechanism model for upward vertical flow for bubbly, slug and annular flow where the flow regime transition were similarly taken from previous work (Taitel et al., 1980; Barnea, 1986; Ansari et al., 1994). The authors developed a large experimental database using water and air as fluids. The model was then tested against other models using the TUFFP. Following the models for vertical upward flow, Tengesdal
et al. (1999) formulated a mechanistic model for vertical upward flow for bubble, dispersed bubble, slug, churn and annular flow. They proposed a new transition model for churn flow, while they took the others from the literature (Ansari et al., 1994; Chokshi et al., 1996). Also, a new hydrodynamic model for churn flow is presented. Finally, they compared their model with field data from the expanded TUFFP, which adds data from the Tulsa University Artificial Lift Projects (TUALP).

For horizontal and near horizontal pipes, Xiao et al. (1990) developed a mechanistic model ($\theta = -15^\circ$ to $15^\circ$) that included four flow regimes, namely stratified, intermittent, annular and dispersed bubble flow. The authors did not perform experiments, but instead gathered data which included large diameter field data (McLeod et al., 1971; Crowley, 1988) and laboratory data (Eaton and Brown, 1965; Payne et al., 1979).

There are several models in the literature that predict flow behavior for all angles of upward flow: $\theta = 0^\circ$ to $90^\circ$. In 1987, Ozon et al. (1987) presented an upward unified model for three flow regimes, bubble flow, intermittent flow and annular flow, and their transitions. They used a big test loop, with up to 30 meter long pipes and experiments were performed with a pressure of up to 50 bar. They compared the model against field data from 90 producing wells, although the properties and characteristics of these wells are not available. Later, Hasan and Kabir (1988a) considered four flow regimes (bubbly, slug, churn and annular), where the flow pattern transitions were based on other work (Orkiszewski, 1967; Aziz et al., 1972; Chierici et al., 1974; Hasan and Kabir, 1988b). The authors performed experiments in vertical and deviated pipes up to $\theta = 58^\circ$, although they gathered other data for lower inclination angles. The model was compared against field data (Griffith et al., 1973) and laboratory experiments Sevingny (1962); Lau (1972); Beggs (1972). The performance of their vertical model was also analyzed in Kabir and Hasan (1990) against field data from Baxendell and Thomas (1961); Orkiszewski (1967); Aziz et al. (1972); Chierici et al. (1974). Kaya et al. (1999) presented a model for bubbly, dispersed bubble, slug, churn and annular flow regimes in highly inclined pipes. They proposed a new bubbly flow transition model, and they used models from the literature for the rest.
(Taitel et al., 1980; Barnea, 1987; Ansari et al., 1994; Tengesdal et al., 1999). Furthermore, a new hydrodynamic model for bubbly flow was also proposed. Similar to Tengesdal et al. (1999), the model was compared against the data from the expanded TUFFP. In the last of the unified upward comprehensive models reviewed, Gomez et al. (2000) presented a model which included stratified, slug, bubble, annular and dispersed bubble flow regimes, and avoided discontinuities by smoothing the transition between the regimes. The model transitions are based on Taitel and Dukler (1976), Taitel et al. (1980) and Barnea (1987). Finally, the model was again compared with laboratory and field measurements (expanded TUFFP, Schmidt (1977), Minami (1983), Alves et al. (1991), Caetano et al. (1992), Felizola and Shoham (1995), Nuland et al. (1997), and data from British Petroleum and Statoil).

The last set of models predict the behavior for all inclination angles, including downward flow: \( \theta = -90^\circ \) to \( 90^\circ \). Petalas and Aziz (2000) presented a unified "mechanistic model applicable to all pipe geometries and fluid properties", including upward and downward flow for bubble, dispersed bubble, annular-mist, stratified, intermittent and froth flow. It incorporated new empirical correlations for liquid/wall and liquid/gas interfacial friction in stratified flow, for the liquid fraction entrained and the interfacial friction in annular-mist flow, and for the distribution coefficient used in the determination of holdup in intermittent flow. Regime transition models were based on Taitel et al. (1980), Barnea et al. (1982), Oliemans et al. (1986), and Barnea (1987). The model was compared with a large database of laboratory and actual field measurements (Petalas and Aziz, 1995). Zhang et al. (2003b,c) proposed a transition criteria for slug, annular, bubbly, stratified, and dispersed bubble flow, and also prediction for their pressure drop and liquid holdup. The flow regime predictions were compared with data from the literature, mainly air/water and air/kerosene experiments (Cheremisinoff, 1977; Mukherjee, 1979; Asali, 1984; Andritsos, 1986; Kouba, 1986; Felizola, 1992).

Employing these methods, the Norwegian OLGA® multiphase transient simulator was proposed. The PLAC code (Black et al., 1990), developed in England a few years later, employs a two-fluid approach too.
<table>
<thead>
<tr>
<th>Source</th>
<th>Flow Pattern Applicability</th>
<th>Inclination Applicability</th>
<th>Transition Model</th>
<th>Evaluated Data</th>
<th>Experiments Performed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fernandes et al. (1983)</td>
<td>Slug</td>
<td>Vertical upward</td>
<td>-</td>
<td>In-house</td>
<td>Water, Air, 90°, 0.05074m, 11.1m, Atmospheric, (v_{SL} = 0 - 3m/s, v_{SG} = 0 - 10m/s)</td>
</tr>
<tr>
<td>Orell and Rembrand (1986)</td>
<td>Slug</td>
<td>Vertical upward</td>
<td>-</td>
<td>Brown et al. (1960); Brown and Geier (1961); Grif- fith and Wallis (1961); Akagawa and Sakaguchi (1966); Sub- botin et al. (1970); Fernandes (1981)</td>
<td>-</td>
</tr>
<tr>
<td>Oss et al. (1987)</td>
<td>Bubbly, Intermittent, Annul- lar (0° to 90°)</td>
<td>In-house</td>
<td>n.a.</td>
<td>Condensate, heavy oil, water</td>
<td>Natural gas, 0° to 90°, 7.62, 15.24cm, 30m, 5-50bar, (q_L = 1.7 \cdot 10^{-4} - 2.3 \cdot 10^{-2} m^3/s ), gas-liquid ratios=0.1-16,000m^3/m^3</td>
</tr>
<tr>
<td>Hasan and Kabir (1988a)</td>
<td>Bubbly, Slug, Churn, Annul- lar (0° to 90°)</td>
<td>Unified upward</td>
<td>Sevingey (1962); Lau (1972); Beggs (1972); Grif- fith et al. (1973)</td>
<td>Water, Air, 58° to 90°, 127mm, 5.5m, Atmospheric</td>
<td>(v_{SL} = 0m/s, v_{SG} = 0 - 0.42m/s)</td>
</tr>
<tr>
<td>Xiao et al. (1990)</td>
<td>Stratified, Intermittent, Annular, Dis- persed Bubble (−15° to 15°)</td>
<td>Horizontal and near horizontal</td>
<td>-</td>
<td>Taitel and Dukler (1976); Barnea et al. (1982)</td>
<td>Eaton and Brown (1965); McLeod et al. (1971); Payne et al. (1979); Crowley (1988)</td>
</tr>
<tr>
<td>Andreussi et al. (1993)</td>
<td>Slug Flow</td>
<td>Horizontal and near horizontal</td>
<td>-</td>
<td>In-house</td>
<td>Water, Air, 0°, 0.3°, ±3°, 18, 50, 90mm, 17.34m, n.a.</td>
</tr>
<tr>
<td>Ansari et al. (1994)</td>
<td>Bubble, Slug, Annular</td>
<td>Vertical upward</td>
<td>TUFFP</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Felizola and Shoham (1995)</td>
<td>Slug Flow</td>
<td>Unified upward</td>
<td>-</td>
<td>In-house</td>
<td>Kerosene, Air, 0° to 90°, 5.1cm, 15m, Atmospheric</td>
</tr>
<tr>
<td>Chokshi et al. (1996)</td>
<td>Bubbly, Slug, Annular</td>
<td>Vertical upward</td>
<td>TUFFP</td>
<td>Water, Air, 90°, 7.6cm, 411m, 1-52 bar</td>
<td>(q_L = 1.5 \cdot 10^{-4} - 7.8 \cdot 10^{-3} m^3/s, q_g = 14 - 920 m^3/s)</td>
</tr>
</tbody>
</table>
Table 2.4: Mechanistic models for multiphase flow (continuation)

<table>
<thead>
<tr>
<th>Flow Pattern Applicability</th>
<th>Inclination Applicability</th>
<th>Transition Model</th>
<th>Evaluated Data</th>
<th>Experiments Performed</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tengesdal et al. (1999)</td>
<td>Vertical upward</td>
<td>Ansari et al. (1994); Chokshi et al. (1996) and in-house</td>
<td>Expanded TUFFP</td>
<td>-</td>
</tr>
<tr>
<td>Kaya et al. (1999)</td>
<td>Unified upward flow</td>
<td>Taitel et al. (1980); Barnea et al. (1992); Ansari et al. (1994) and in-house</td>
<td>Expanded TUFFP</td>
<td>-</td>
</tr>
<tr>
<td>Petalas and Aziz (2000)</td>
<td>Unified upward and downward (-90° to 90°)</td>
<td>Taitel et al. (1980); Barnea et al. (1982); Olemans et al. (1986); Barnea (1987)</td>
<td>Petalas and Aziz (1995)</td>
<td>-</td>
</tr>
<tr>
<td>Gomez et al. (2000)</td>
<td>Unified upward (0° to 90°)</td>
<td>Taitel and Dukler (1976); Taitel et al. (1980); Barnea (1987)</td>
<td>TUFFP and Schmidt (1977); Minami (1983); Alves et al. (1991); Caetano et al. (1992); Feilzola and Shoham (1995); Nurlend et al. (1997)</td>
<td>-</td>
</tr>
<tr>
<td>Abdul-Majeed and Al-Mashat (2000)</td>
<td>Unified upward (0° to 90°)</td>
<td>TUFFP and Schmidt (1977); Feilzola (1992)</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Issa and Kempf (2003)</td>
<td>Horizontal and near horizontal</td>
<td>WASP at Imperial College and others</td>
<td>Water Air 0°, ±1.5° 7.8cm 36, 37m n.a.</td>
<td>-</td>
</tr>
<tr>
<td>Zhang et al. (2003b,c)</td>
<td>Unified upward and downward (-90° to 90°)</td>
<td>Taitel et al. (1980); Grolman (1994); Zhang et al. (2003a)</td>
<td>Cheremisinoff (1977); Mukherjee (1979); Asali (1984); Andritsos (1986); Kouba (1986); Feilzola (1992)</td>
<td>-</td>
</tr>
</tbody>
</table>

Inclination Angle: -
Pipe Diameter: -
Length: -
P_h: -
Flow Rate: -
Unfortunately these approaches do not give accurate predictions of the bottomhole flowing pressure. Also, the empirical approach works relatively well in oil wells, but not in gas wells. The two-fluid approaches give reasonable results in both oil and gas wells. For example, the model of Ansari et al. (1994) can reproduce 62% of the pressure drop for oil wells with ±6% error, and 68% of the pressure drop data in gas wells with ±15% error (Brill and Mukherjee, 1999). Salim and Stanislav (1994) compared methods that describe the flow of gas/liquid mixture in wells exhibiting mostly annular/mist-flow pattern, concluding that correlations from Duns and Ros (1963) and Orkiszewski (1967) appeared to be less efficient than mechanistic models. Brill and Mukherjee (1999) also pointed out some of the existing shortcomings, for example that there is no prediction of simultaneous flow of gas, oil, and water in wellbores. Fazeli and Vatani (2006) compared different closure relations (Taitel and Dukler, 1976; Baker et al., 1988; Petalas and Aziz, 2000; Gomez et al., 2000), reaching the conclusion that Petalas and Aziz (2000) model seemed more reliable in liquid holdup calculation while Gomez et al. (2000) model was more accurate on pressure drop estimation.

In the following chapter, the mechanistic models of Orell andRembrand (1986), Ansari et al. (1994) and Petalas and Aziz (2000) are studied in detail in order to obtain which of the closure relations that they use are the dominant ones. The objective of this project is to improve the model predictions through an improvement of the closure relations.
2.4.2 Nuclear industry

In the nuclear power industry, two-phase flow is critical as nuclear reactors use water boiling to remove heat from the reactor core. Thus, two-phase flow modeling has been deeply investigated. Here, only some representative examples of the vast amount of correlations that exist are mentioned.

As mentioned before, it was Zuber and Findlay (1965), researchers in the nuclear industry, who developed the widely used drift-flux model to calculate void fraction. Later, the well-known EPRI correlation of Chexal et al. (1992), referred as the Chexal-Lellouche correlation, was presented to predict the void fraction for a wide range of fluids, flow regimes and geometries. The authors tested the correlation against steady-state two-phase flow data that covered a wide range of thermodynamic conditions and geometries typical of Pressurized Water Reactor (PWR) and Boiling Water Reactor (BWR) fuel assemblies and for pipes up to 0.45m in diameter. The correlation did not depend on flow regime maps or spline fitting. Chexal et al. (1991) analyzed eight drift-flux models for predicting the void fraction, and concluded that the Chexal-Lellouche correlation, together with the correlations from Dix (1971) and Punches (1977), provided the best overall predictions of all the void fraction data.

Furthermore, important parameters such as the critical heat flux are calculated with two-phase flow models. Okawa et al. (2004) presented a model to predict that in annular regime in various vertical channels. In their model, quantities such as deposition and entrainment rates of droplets were evaluated with the correlations based on experimental data.

Finally, the pressure gradient is another key variable to calculate. The Friedel correlation (Friedel, 1979), who used a database of 25,000 points for both horizontal and vertical upward flow, has been amply employed. It should be noted that these models mentioned herein are only some representative examples of the vast amount of correlations that exist.
Chapter 3

Sensitivity Study

3.1 Introduction

The current simulation tools to predict multiphase flows, the mechanistic or phenomenological models, require closure relations to complete the conservation equations of mass, momentum, and energy of each phase, so that flow parameters such as liquid holdup (void fraction) and pressure drop can be predicted. Herein, a sensitivity analysis of three different models published in literature (Orell and Rembrand, 1986; Ansari et al., 1994; Petalas and Aziz, 2000) is performed in order to determine how these closure relations impact the outcome. It is important to note that they are from different research groups. The models and sensitivity analysis are implemented in MATLAB® (2013). The results show that the Taylor bubble terminal velocity is the dominant closure relation. Thus, the following chapters are focused on its improvement through CMFD simulations.

In this chapter, first the sensitivity analysis procedure is described. Then, the mechanistic models studied are described, and finally the sensitivity results are shown. It should be noted that the notation of the mechanistic models have been slightly changed to present them consistently in this document.
3.2 Mathematical procedure

The figures of merit, which we treat as the dependent variables, are the slug unit liquid holdup, $H_{SU}$, and the pressure gradient, $dp/dL$. The closure relations are the extra equations different from the conservation equations needed to close the model’s set of variables. In our analysis, the variables obtained with the closure relations are treated as independent variables. That is,

$$H_{SU} = f(x_1, x_2, ..., x_n),$$

$$\frac{dp}{dL} = g(x_1, x_2, ..., x_n),$$

where $x_1, x_2, ..., x_n$ are the $n$ closure relations used in each model. The sensitivity coefficients are calculated as

$$\phi_{f,i} = \frac{\partial f(x_1, x_2, ..., x_n)}{\partial x_i} \cdot \frac{x_i}{f(x_1, x_2, ..., x_n)},$$

$$\phi_{g,i} = \frac{\partial g(x_1, x_2, ..., x_n)}{\partial x_i} \cdot \frac{x_i}{g(x_1, x_2, ..., x_n)},$$

for $i = 1, ..., n$, and measure the change in the figure of merit prediction, $H_{SU}$ for $\phi_{f,i}$ and $dp/dL$ for $\phi_{g,i}$, due to the variation of the closure relation $x_i$. Previous partial derivatives of $f$ and $g$ with respect to closure relation $x_i$ cannot be calculated analytically since the functions $f$ and $g$ are not explicit. Thus, we approximate the derivatives as finite differences:

$$\phi_{f,i} \approx \frac{\Delta f(x_1, x_2, ..., x_n)}{\Delta x_i} \cdot \frac{x_i}{f(x_1, x_2, ..., x_n)},$$

$$\phi_{g,i} \approx \frac{\Delta g(x_1, x_2, ..., x_n)}{\Delta x_i} \cdot \frac{x_i}{g(x_1, x_2, ..., x_n)}.$$

The closure relations $x_i, i = 1, ..., n$, are dependent on the case input values: superficial velocities, tube geometry and fluid properties. Thus, the closure relations are first calculated with those nominal case values, and then modified to obtain the sensitivity coefficients. In
this case, a 2nd-order central difference approximation is used. That is,

\[
\frac{\Delta f(x_1, x_2, ..., x_n)}{\Delta x_i} = \frac{f(x_1, x_2, ..., (1 + \epsilon) \cdot x_i, ..., x_n) - f(x_1, x_2, ..., (1 - \epsilon) \cdot x_i, ..., x_n)}{(1 + \epsilon) \cdot x_i - (1 - \epsilon) \cdot x_i}
\]

\[
= \frac{f(x_1, x_2, ..., (1 + \epsilon) \cdot x_i, ..., x_n) - f(x_1, x_2, ..., (1 - \epsilon) \cdot x_i, ..., x_n)}{2\epsilon x_i}, \quad (3.4)
\]

where \( \epsilon \) is a small amount. In the present work, the sensitivity coefficients converged for \( \epsilon = 0.001 \). \( \Delta g(x_1, x_2, ..., x_n)/\Delta x_i \) is obtained similarly. If equation 3.4 is used in equations 3.3, then

\[
\phi_{f,i} = \frac{f(x_1, x_2, ..., (1 + \epsilon) \cdot x_i, ..., x_n) - f(x_1, x_2, ..., (1 - \epsilon) \cdot x_i, ..., x_n)}{2\epsilon f(x_1, x_2, ..., x_n)} \cdot \frac{1}{f(x_1, x_2, ..., x_n)}, \quad (3.5a)
\]

\[
\phi_{g,i} = \frac{g(x_1, x_2, ..., (1 + \epsilon) \cdot x_i, ..., x_n) - g(x_1, x_2, ..., (1 - \epsilon) \cdot x_i, ..., x_n)}{2\epsilon g(x_1, x_2, ..., x_n)} \cdot \frac{1}{g(x_1, x_2, ..., x_n)}. \quad (3.5b)
\]

The mechanistic models studied (Orell and Rembrand, 1986; Ansari et al., 1994; Petalas and Aziz, 2000) are described in the following section. We analyzed these models because they were developed in different research groups, and comprised different mechanistic model types described in the previous chapter: an upward vertical slug flow model (Orell and Rembrand, 1986), a comprehensive upward vertical model that includes other flow regimes different from slug flow (Ansari et al., 1994), and a comprehensive unified model that includes other flow regimes, and upward and downward flow (Petalas and Aziz, 2000).

### 3.3 Description of slug flow models

Slug flow mechanistic models represent the flow regime as a sequence of fundamental units, also called slug units. Each unit contains a Taylor bubble and a liquid slug (see figure 1-3 of chapter 1). The unknown variables include the Taylor bubble velocity, \( v_{TB} \), the Taylor bubble gas velocity, \( v_{gTB} \), the Taylor bubble liquid velocity, \( v_{LTB} \), the liquid slug gas velocity, \( v_{gLS} \), the liquid slug liquid velocity, \( v_{LLS} \), the Taylor bubble void fraction, \( \alpha_{TB} \), the liquid slug void fraction, \( \alpha_{LS} \), the Taylor bubble length, \( L_{TB} \), the liquid slug length, \( L_{LS} \), and the
pressure drop in the Taylor bubble and liquid slug, \( (dp/dL)_{TB} \) and \( (dp/dL)_{LS} \), respectively. Mechanistic models differ from each other in the assumptions made to simplify the model, in the closure relations used to obtain a closed set of equations and in the flow regime transition models. Here, we describe and analyze three different models: Orell and Rembrand (1986), Ansari et al. (1994) and Petalas and Aziz (2000).

### 3.3.1 Orell and Rembrand (1986)

Orell and Rembrand (1986) developed a hydrodynamic model for vertical upward gas-liquid turbulent slug flow. The model includes seven unknowns\(^1\): the Taylor bubble velocity, \( v_{TB} \); the Taylor bubble film thickness, \( h \); the velocity of the liquid film, \( v_{LTB} \); the film friction factor, \( f_f \); the liquid holdup in the liquid slug, \( H_{LS} \); total slug unit liquid holdup, \( H_{SU} \); and the Taylor bubble length over the slug unit length ratio, \( \beta = L_{TB}/L_{SU} \). The seven equations used comprise three mass balances, one friction correlation, one force balance, and two closure relations. A brief description of the model is given here, although the reader is referred to the article for a more detailed description. The basic assumptions of the model are:

1. The slug flow is one-dimensional, steady state fully developed.
2. The flow regime for the liquid in both the slug and the film is turbulent.
3. There is no slip between the bubble swarm and the liquid in the liquid slug region.
4. The liquid film contains no bubbles.
5. The Taylor bubble is approximated by a cylinder of constant diameter.

The two closure relations calculate (i) the Taylor bubble velocity, \( v_{TB} \), and (ii) the liquid slug liquid holdup, \( H_{LS} \).

\(^1\)Pressure drop, \( dp/dL \), is not considered an unknown here because it is obtained with the typical pressure drop equation once the other model variables are obtained, as it is shown later.
First, the Taylor bubble velocity, \( v_{TB} \), is modeled as a superposition of the bubble rise velocity in a stagnant liquid and the contribution of the flowing liquid, based on the proposition of Nicklin et al. (1962). Thus,

\[
v_{TB} = 1.2v_m + 0.35\sqrt{gd}, \tag{3.6}
\]

where \( g \) is gravity, and \( d \) is the pipe diameter.

Secondly, the liquid slug liquid holdup, \( H_{LS} \), is obtained using geometrical considerations and experimental observations. The resultant equation is

\[
H_{LS} = \frac{4h(v_{LTB} + v_{TB})}{0.6C_Wd\sqrt{(v_{LTB} + v_{TB})^2 - 2g((0.6C_W(d/2)^2 - h \cdot d)^{1/2} + d)}}, \tag{3.7}
\]

where \( C_W = 0.29 \) is the fractional tube cross section in which the local liquid velocity is lower than \( v_m \) assuming turbulent flow in the liquid slug.

Once the model variables are calculated, the figures of merit are computed. The liquid holdup in the slug unit, \( H_{SU} \), is calculated as

\[
H_{SU} = \frac{4hL_{TB}}{dL_{SU}} + H_{LS}\left(1 - \frac{L_{TB}}{L_{SU}}\right). \tag{3.8}
\]

Regarding the pressure gradient, \( dp/dL \), the pressure is modeled constant along the Taylor bubble region, i.e., the pressure drop due to friction of the liquid film with the pipe wall is essentially balanced by the gravitational pressure drop of the two-phase mixture. Thus, only the liquid slug pressure drop is calculated:

\[
\frac{dp}{dL} = \left(g\rho_{LS} + \frac{2f_{LS}\rho_{LS}v_m^2}{d}\right)\frac{L_{LS}}{L_{SU}}, \tag{3.9}
\]

where \( \rho_{LS} \) is the mixture density in the liquid slug, \( \rho_{LS} = H_{LS}\rho_L + (1 - H_{LS})\rho_y \).

Figures 3-1 to 3-3 reproduce satisfactorily the results provided by Orell and Rembrand (1986) for air/water mixture in a pipe of \( d = 0.0276 \)m (table 3.1). Figure 3-1 depicts the ratio of Taylor bubble length over the slug unit length, \( L_{TB}/L_{SU} \), for four different liquid
superficial velocities, $v_{SL}$, with respect to the gas superficial velocity, $v_{SG}$ (a), and for four different mixture velocities, $v_m$, with respect to the ratio of gas over total volumetric flow, $Q_g/Q_T$ (b). At a fixed liquid superficial velocity, the length ratio increases with higher gas flow as the Taylor bubble void fraction is higher than the liquid slug one. Also, at a fixed gas superficial velocity, the length ratio decreases with higher liquid flow as the liquid holdup of the liquid slug is higher than that of the Taylor bubble. Furthermore, it is interesting to note that, for a fixed ratio of gas over the total superficial velocity, the length ratio increases with increasing mixture velocity, $v_m$: Taylor bubble length tends to increase with fluid flow, evolving progressively to churn flow. Figure 3-2 shows the slug unit void fraction, $\alpha_{SU}$, with respect to the same variables $v_{SG}$ (a) and $Q_g/Q_T$ (b). The trends follow by the the void fraction, $\alpha_{SU}$, are the same ones of the length ratio, $L_{TB}/L_{SU}$. Finally, figure 3-3 depicts the pressure drop over the slug unit length, $dp/dL$, for five different liquid superficial velocities, $v_{SL}$, with respect to the gas superficial velocity, $v_{SG}$. As expected, pressure drop increases with liquid superficial velocity ($\beta$ is reduced and equation 3.9 increases), and it decreases with gas superficial velocity (in this case, $\beta$ increases and the overall effect on equation 3.9 is to decrease).

Table 3.1: Air/water mixture properties provided by Orell and Rembrand (1986)

<table>
<thead>
<tr>
<th>$d$ [m]</th>
<th>$\rho_g$ [kg/m$^3$]</th>
<th>$\rho_L$ [kg/m$^3$]</th>
<th>$\mu_g$ [Pa·s]</th>
<th>$\mu_L$ [Pa·s]</th>
<th>$\sigma$ [N/m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0276</td>
<td>1.2041</td>
<td>999</td>
<td>1.827$\cdot$10$^{-5}$</td>
<td>1$\cdot$10$^{-3}$</td>
<td>7.1971$\cdot$10$^{-2}$</td>
</tr>
</tbody>
</table>

3.3.2 Ansari et al. (1994)

The last mechanistic model studied is provided by Ansari et al. (1994), which applies to upward two-phase flow. The model is composed by a flow pattern prediction model and a set of independent mechanistic models that calculate the liquid holdup and pressure drop in bubble, slug and annular flow. The slug flow model is the one of Sylvester (1987), which is a simplified version of the model presented by Fernandes et al. (1983). It has eight unknowns: the gas velocity in the Taylor bubble, $v_{gTB}$; the liquid film velocity in the Taylor bubble,
Figure 3-1: Comparison of theoretical values of the ratio of Taylor bubble length over the slug unit length, $L_{TB}/L_{SU}$, for an air/water mixture (table 3.1) and different superficial velocities reported by Orell and Rembrand (1986) (circled solid line) with the results obtained in the in-house implementation (dash-dotted line).

Figure 3-2: Comparison of theoretical values of the total void fraction in the slug unit, $\alpha_{SU}$, for an air/water mixture (table 3.1) and different superficial velocities reported by Orell and Rembrand (1986) (circled solid line) with the results obtained in the in-house implementation (dash-dotted line).

$v_{LTB}$; the bubbles’ velocity in the liquid slug, $v_{gLS}$; the liquid velocity in the liquid slug, $v_{LLS}$; the Taylor bubble velocity, $v_{TB}$; the void fraction in the Taylor bubble, $\alpha_{TB}$; the liquid holdup in the liquid slug, $H_{LS}$; and the ratio of the Taylor bubble length over the slug unit length, $\beta$. The model uses four mass conservation equations (overall gas and liquid mass...
balances, and mass balances for liquid and gas from the liquid slug to the Taylor bubble) and four closure relations. The closure relations calculate (i) the Taylor bubble velocity, \( v_{TB} \), (ii) the velocity of the gas bubbles in the liquid slug, \( v_{gLS} \), (iii) the velocity of the falling film, \( v_{LTB} \), and (iv) the liquid slug liquid holdup, \( H_{LS} \).

As in the previous models, the Taylor bubble velocity, \( v_{TB} \), is calculated first:

\[
v_{TB} = 1.2 v_m + 0.35 \sqrt{\frac{gd(p_L - p_g)}{\rho_L}}. \tag{3.10}
\]

Secondly, the velocity of the gas bubbles in the liquid slug, \( v_{gLS} \), is similarly obtained through

\[
v_{gLS} = 1.2 v_m + 1.52 \left( \frac{g\sigma_L(p_L - p_g)}{\rho_L^2} \right)^{1/4} \sqrt{H_{LS}}. \tag{3.11}
\]

In third place, the velocity of the falling film, \( v_{LTB} \), is obtained based on the correlation of Brötz (1954),

\[
v_{LTB} = 9.916 \sqrt{gd(1 - \sqrt{\alpha_{TB}})}. \tag{3.12}
\]

Finally, the liquid slug liquid holdup, \( H_{LS} \), is obtained through the following drift model.
proposed by Sylvester (1987), where the coefficients are empirically obtained:

\[ H_{LS} = 1 - \frac{v_{sg}}{0.425 + 2.65v_m} \]  

(3.13)

Similarly as before, the slug unit liquid holdup is calculated using equation 3.22c. In this model, the pressure drop in the slug unit, \( \frac{dp}{dL} \), comprises two components, gravitational and frictional,

\[ \left( \frac{dp}{dL} \right) = \left( \frac{dp}{dL} \right)_g + \left( \frac{dp}{dL} \right)_f. \]  

(3.14)

The gravitational component is calculated as

\[ \left( \frac{dp}{dL} \right)_g = g (\beta \rho_g + (1 - \beta) \rho_{LS}), \]  

(3.15)

where \( \rho_{LS} = \rho_L H_{LS} + \rho_g (1 - H_{LS}) \). Secondly, the frictional component is calculated based only on the friction in the liquid slug,

\[ \left( \frac{dp}{dL} \right)_f = f_{LS} \rho_{LS} v_m^2 \frac{1 - \beta}{2d}, \]  

(3.16)

where the liquid slug friction factor, \( f_{LS} \), is calculated based on the liquid slug Reynolds number,

\[ Re_{LS} = \frac{\rho_{LS} v_m d}{\mu_{LS}}, \]  

(3.17)

where \( \mu_{LS} \) is the liquid slug viscosity, \( \mu_{LS} = \mu_L H_{LS} + \mu_g (1 - H_{LS}) \).

### 3.3.3 Petalas and Aziz (2000)

Petalas and Aziz (2000) presented a unified mechanistic model for two-phase flow applicable to all round pipe geometries and fluid properties. In the article, new empirical correlations are proposed for liquid/wall and liquid gas interfacial friction in stratified flow, for the liquid fraction entrained and the interfacial friction in annular-mist flow, and for the distribution coefficient used in the determination of liquid holdup in intermittent flow. Here,
the slug flow pattern prediction is described first, and then the equations used in the slug flow model are introduced.

The transition from dispersed bubble to slug flow is based on the proposition of Barnea (1986), where it occurs when the liquid holdup in the liquid slug, $H_{LS}$, is less than the value associated with the maximum volumetric density of the dispersed bubbles:

$$H_{LS} < 0.48,$$  \hspace{1cm} (3.18)

where $H_{LS}$ is calculated by the correlation of Gregory et al. (1978):

$$H_{LS} = \frac{1}{1 + (v_m/8.66)^{1.39}}.$$  \hspace{1cm} (3.19)

On the other hand, at low liquid superficial velocities, not enough liquid may be available for slug formation and transition to annular flow may occur (Barnea, 1987). This happens when

$$H_{SU} \leq 0.24,$$  \hspace{1cm} (3.20)

where $H_{SU}$ is the slug unit liquid holdup, calculated by

$$H_{SU} = \frac{H_{LS}v_{TB} + v_{gLS}(1 - H_{LS}) - v_{sg}}{v_{TB}},$$  \hspace{1cm} (3.21)

where $v_{gLS}$ is the bubble gas velocity in the liquid slug. The latter equation is obtained combining the following overall gas mass balance, gas mass balance from the liquid slug to Taylor bubble, and the definition of slug unit liquid holdup:

$$v_{sg} = \beta v_{gTB}(1 - H_{TB}) + (1 - \beta)v_{gLS}(1 - H_{LS}),$$  \hspace{1cm} (3.22a)

$$(v_{TB} - v_{gLS})(1 - H_{LS}) = (v_{TB} - v_{gTB})(1 - H_{TB}),$$  \hspace{1cm} (3.22b)

$$H_{SU} = \beta H_{TB} + (1 - \beta)H_{LS},$$  \hspace{1cm} (3.22c)

respectively.
Moreover, the elongated bubble flow is defined in the article as the portion of intermittent flow for which the liquid slug contains no dispersed bubbles, different from slug flow. This condition is represented by

\[ H_{SU} \geq 0.90. \]  

(3.23)

The slug flow model consists of eight unknowns: the Taylor bubble velocity, \( v_{TB} \); the gas bubble velocity in the liquid slug, \( v_{gLS} \); the liquid film velocity in the Taylor bubble, \( v_{LTB} \); the liquid holdup in the liquid slug, \( H_{LS} \); the liquid holdup in the Taylor bubble, \( H_{TB} \); the slug unit liquid holdup, \( H_{SU} \); the ratio of the Taylor bubble length over the slug unit length, \( \beta \); and the liquid fraction entrained inside the Taylor bubble, \( FE \). To solve these unknowns, the model uses three mass balance equations and five closure relations. The closure relations calculate (i) the Taylor bubble velocity, \( v_{TB} \), (ii) the liquid holdup of the liquid slug, \( H_{LS} \), (iii) the dispersed bubbles’ velocity in the liquid slug, \( v_{gLS} \), (iv) the Taylor bubble length over the slug unit length ratio, \( \beta \), and (v) the entrainment factor, \( FE \).

First, similar to Orell and Rembrand (1986), the Taylor bubble velocity, \( v_{TB} \), is calculated based on the proposition of Nicklin et al. (1962):

\[ v_{TB} = C_0 v_m + v_d, \]  

(3.24)

where the parameter \( C_0 \) is a distribution parameter related to the velocity profile, and \( v_d \) is the so-called Taylor bubble drift velocity which is the bubble velocity in stagnant liquid. Since the model is unified, different from the model of Orell and Rembrand (1986), both \( C_0 \) and \( v_d \) account for the inclination angle. The distribution parameter, \( C_0 \), is obtained with an empirical correlation,

\[ C_0 = (1.64 + 0.12 \sin \theta) R_{e_{mL}}^{-0.031}, \]  

(3.25)

where \( \theta \) is the inclination angle with respect to the horizontal, and the Reynolds number \( R_{e_{mL}} \) is

\[ R_{e_{mL}} = \frac{\rho_L v_m d}{\mu_L}. \]  

(3.26)
The Taylor bubble drift velocity $v_d$ is calculated from the correlation of Zukoski (1966),

$$v_d = v_{d,\infty} \cdot \min \left( 0.316 \sqrt{Re_{\infty}}, 1 \right), \quad (3.27)$$

where

$$Re_{\infty} = \frac{\rho_L v_{d,\infty} d}{2 \mu_L}, \quad (3.28)$$

and $v_{d,\infty}$ is the velocity given by the correlation of Bendiksen (1984) at high Reynolds numbers:

$$v_{d,\infty} = v_{h,d,\infty} \cos \theta + v_{v,d,\infty} \sin \theta, \quad (3.29)$$

where $v_{h,d,\infty}$ and $v_{v,d,\infty}$ are the horizontal and vertical Taylor bubble drift velocities, respectively. $v_{h,d,\infty}$ is given by Weber (1981) as

$$v_{h,d,\infty} = \left( 0.54 - \frac{1.76}{Bo^{0.56}} \right) \sqrt{\frac{gd(\rho_L - \rho_g)}{\rho_L}}, \quad (3.30)$$

where $Bo$ is the Bond number,

$$Bo = \frac{\rho_L - \rho_g}{\sigma} gd^2. \quad (3.31)$$

The vertical Taylor bubble drift velocity, $v_{v,d,\infty}$, is obtained from a modified form of the correlation of Wallis (1969),

$$v_{v,d,\infty} = 0.345 \left( 1 - e^{-\zeta} \right) \sqrt{\frac{gd(\rho_L - \rho_g)}{\rho_L}}, \quad (3.32)$$

where the coefficient $\zeta$ is

$$\zeta = Bo \cdot e^{3.278 - 1.424 \ln Bo}. \quad (3.33)$$

The second closure relation to calculate the liquid slug liquid holdup, $H_{LS}$, is equation 3.19.
In the third place, the bubbles' velocity in the liquid slug, $v_{gLs}$, is calculated as

$$v_{gLs} = C_0 v_m + v_b,$$  \hspace{1cm} (3.34)

where the bubbles drift velocity, $v_b$, is obtained using the expression of Harmathy (1960):

$$v_b = 1.53 \left( \frac{g (\rho_L - \rho_g) \sigma}{\rho_L^2} \right)^{1/4} \sin \theta.$$  \hspace{1cm} (3.35)

In the fourth place, the ratio of the Taylor bubble length over the slug unit length, $\beta$, is calculated from

$$\beta = \frac{L_{TB}}{L_{SU}} = 1 - \min \left( \left( \frac{v_{SL}}{v_m} \right)^{0.75 - H_{SU}}, 1 \right).$$  \hspace{1cm} (3.36)

Finally, the entrainment factor, $FE$, is obtained using the following empirical correlation,

$$\frac{FE}{1 - FE} = 0.735 N_B^{0.074} \left( \frac{v_{SL}}{v_{SL}} \right)^{0.2},$$ \hspace{1cm} (3.37)

where $N_B$ is a dimensionless number defined as

$$N_B = \frac{\mu_L^2 v_{SL} \rho_g}{\sigma^2 \rho_L}.$$  \hspace{1cm} (3.38)

Once the eight unknowns of the model are calculated, the pressure gradient, $dp/dL$, can be computed. It is divided in three terms: the gravitational term, the frictional pressure drop in the liquid slug, and the frictional pressure drop in the Taylor bubble,

$$- \left( \frac{dp}{dL} \right) = \rho_m \sin \theta + (1 - \beta) \left( \frac{dp}{dL} \right)_{f_{LS}} + \beta \left( \frac{dp}{dL} \right)_{f_{TB}},$$  \hspace{1cm} (3.39)

where $\rho_m = H_{SU} \rho_L + (1 - H_{SU}) \rho_g$. The liquid slug frictional pressure gradient is calculated by

$$\left( \frac{dp}{dL} \right)_{f_{LS}} = \frac{2 f_{mL} v_m^2 \rho_m}{d},$$ \hspace{1cm} (3.40)

where the friction factor $f_{mL}$ is based on the Reynolds number given in equation 3.26.
The frictional pressure drop in the Taylor bubble is based on annular-mist flow if the non-dimensional film thickness, \( \bar{h} = h/d \), is higher than \( \bar{h} > 1 \cdot 10^{-4} \):

\[
\left( \frac{dp}{dL} \right)_{fTB} = \frac{4\tau_{wL}}{d},
\]

(3.41)

where \( \tau_{wL} \) is the wall shear stress,

\[
\tau_{wL} = \frac{f_f(-v_{LTB}^2) \rho_L}{2},
\]

(3.42)

where \( f_f \) is a friction factor based on the following Reynolds number,

\[
Re_f = \frac{\rho_L v_{LTB} d}{\mu_L}.
\]

(3.43)

Otherwise, if \( \bar{h} \leq 1 \cdot 10^{-4} \), an homogeneous model with slip is used to calculate \( (dp/dL)_{fTB} \),

\[
\left( \frac{dp}{dL} \right)_{fTB} = \frac{2f_m v_m^2 \rho_m}{d},
\]

(3.44)

where \( f_m \) is a friction factor based on the following Reynolds number,

\[
Re_m = \frac{\rho_m v_m d}{\mu_m},
\]

(3.45)

where \( \mu_m \) is the mixture viscosity calculated as \( \mu_m = H_{SU} \mu_L + (1 - H_{SU}) \mu_g \).

In order to validate our implementation, the results provided by Petalas and Aziz (2000) for a gas/oil mixture, whose properties and geometry are shown in table 3.2, are reproduced in figure 3-4.

Table 3.2: Gas/oil mixture properties provided by Petalas and Aziz (2000)

<table>
<thead>
<tr>
<th>( \theta ) [°]</th>
<th>( d ) [m]</th>
<th>( \rho_g ) [kg/m³]</th>
<th>( \rho_L ) [kg/m³]</th>
<th>( \mu_g ) [Pa·s]</th>
<th>( \mu_L ) [Pa·s]</th>
<th>( \sigma ) [N/m]</th>
<th>Abs. pipe roughness [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.16</td>
<td>130.4</td>
<td>841.4</td>
<td>1.8·10⁻⁵</td>
<td>2.76·10⁻³</td>
<td>2.0·10⁻²</td>
<td>3.05·10⁻³</td>
</tr>
</tbody>
</table>
3.4 Sensitivity results

This section shows the sensitivity results obtained following the procedure described in section 3.2. First, a case study representative of a typical Kuwaiti well, whose properties and pipes geometry are shown in table 3.3, is performed and validated with our collaborators from the Kuwait University. Later, we analyze more cases that cover the fluid property ranges studied in more detail in chapter 6 and 7.

The sensitivity results for the Kuwaiti well, shown in table 3.4, determine that the Taylor
bubble velocity, $v_{TB}$, is the dominant closure relation in Orell and Rembrand (1986), affects strongly the outcome in the mechanistic model of Petalas and Aziz (2000) together with $H_{LS}$ and $v_{gLS}$ for $dp/dL$ and $v_{gLS}$ for $H_{SU}$, and finally is dominant together with $v_{gLS}$ in that of Ansari et al. (1994). Since each model has different assumptions that relate the variables differently, it is interesting to analyze these results closer.

First, we look at the coefficients of the model of Orell and Rembrand (1986). The Taylor bubble velocity sensitivity coefficients are positive for both $H_{SU}$ and $dp/dL$. When the Taylor bubble velocity, $v_{TB}$, increases, the gas velocity in the Taylor bubble region increases, it occupies less sectional area, and thus the Taylor bubble liquid holdup, $H_{TB}$, increases. Although there is a redistribution of the Taylor bubble and liquid slug lengths, reducing $\beta$, the augmentation of $H_{TB}$ makes the slug unit holdup, $H_{SU}$, to increase. Regarding the pressure drop, $dp/dL$, as $\beta$ decreases while the other terms of equation 3.9 remain constant, $dp/dL$ increases with $v_{TB}$.

For the liquid slug holdup, $H_{LS}$, both coefficients are also positive. When $H_{LS}$ increases, $H_{TB}$ remains constant as it only depends on $v_{TB}$. Thus, $\beta$ increases based on the following equation,

$$\beta = \frac{v_{sg} - (1 - H_{LS})v_m}{v_{TB}(1 - H_{TB}) - (1 - H_{LS})v_m}.$$  \hspace{1cm} (3.46)

Since both $H_{LS}$ and $\beta$ increase, so does $H_{SU}$. On the other hand, $\rho_{LS}$ increases by definition, and it also counterbalances the augmentation of $\beta$ while other terms of equation 3.9 remain constant, increasing the value of $dp/dL$.

The model of Ansari et al. (1994) is solved with an iterative procedure due to the high nonlinearity of the system of equations. First, the Taylor bubble velocity, $v_{TB}$, generates similar effects as before: its increase causes $H_{TB}$ to increase and so does $H_{SU}$, where in this case the reduction of $\beta$ does not balance the other. Since $\beta$ decreases, the gravitational component of the pressure drop, $(dp/dL)_g$, increases as the liquid slug fraction is more important, and $\rho_{LS} > \rho_g$. Furthermore, the friction component in the liquid slug, $(dp/dL)_f$, also increases because of the same reason: $\beta$ decreases while the other components in equation 3.16 remain constant.
Secondly, the sensitivity coefficients of liquid slug liquid holdup, $H_{LS}$, presents different signs. First, its augmentation produces a redistribution in the slug unit liquid, and $H_{TB}$ and $\beta$ increases, with an overall increase of the slug unit liquid slug, $H_{SU}$. On the other hand, when $H_{LS}$ increases, the increment in $\beta$ reduces both $(dp/dL)_g$ (even though $\rho_{LS}$ increases), and $(dp/dL)_f$ (despite $f_{LS}$ also increases slightly).

In the third closure relation, the augmentation of the velocity of the dispersed bubbles in the liquid slug, $v_{gLS}$, makes the gas in the liquid slug to occupy less, which, while maintaining $H_{LS}$ constant, absorbs gas from the Taylor bubble and thus reduces $\beta$ at the same time that $H_{TB}$ increases. The overall effect is an increase of the slug unit liquid slug, $H_{SU}$. Regarding the pressure drop, as $\beta$ gets smaller, both $(dp/dL)_g$ and $(dp/dL)_f$ increase due to a higher proportion of the liquid slug while the other terms remain constant.

Finally, the film velocity, $v_{LTB}$, decreases slightly the slug unit liquid holdup, $H_{SU}$: its increment reduces $H_{TB}$ more significantly than $\beta$. Furthermore, it affects the pressure drop more significantly: similar to the previous closure relation, the reduction in $\beta$ causes both $(dp/dL)_g$ and $(dp/dL)_f$ to increase as the other terms remain constant.

Lastly, the results obtained with the model of Petalas and Aziz (2000) are discussed. Similarly as before, when $v_{TB}$ increases, the gas velocity in the Taylor bubble region increases, it occupies less sectional area, and thus the slug unit liquid holdup, $H_{SU}$, increases, directly from equation 3.21. On the other hand, the pressure drop, $dp/dL$, increases too. As $\rho_m$ increases with $H_{SU}$ by definition, it follows that the gravitational and the liquid slug frictional pressure drop terms also augments. Moreover, the frictional pressure drop in the Taylor bubble decreases in absolute value as the film velocity, $v_{LTB}$, decreases and the friction factor, $f_f$, increases ($\tilde{h} > 1 \cdot 10^{-4}$), and, since it is negative, contributes to the increase in overall pressure drop.

Secondly, looking at the liquid slug holdup, $H_{LS}$, the behavior is different than in the model of Orell and Rembrand (1986): in this case, sensitivity coefficients are both negative. For this case, since $v_{gLS}$ is slightly higher than $v_{TB}$, $H_{SU}$ decreases based on equation 3.21. Following this, $\rho_m$ decreases as well, and thus the pressure drop, $dp/dL$. 

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In the third place, as the velocity of the dispersed bubbles in the liquid slug, \( v_{gLS} \), increases, it follows that so does \( H_{SU} \) based on equation 3.21. As a consequence, \( \rho_m \) and thus the pressure drop, \( dp/dL \), increase.

In the fourth place, we analyze the ratio of the Taylor bubble over the liquid slug lengths, \( \beta \). It is clear that it does not affect equation 3.21, and thus the sensitivity coefficient is zero for \( H_{SU} \). On the other hand, the coefficient of \( \beta \) is positive for \( dp/dL \): as \( \beta \) increases and \( H_{TB} \) remains constant, the film velocity, \( v_{LTB} \), decreases and, as before, \( f_f \) increases. Thus, the frictional pressure drop in the Taylor bubble decreases in absolute terms, contributing to increase the pressure drop. As \( \beta \) decreases while the gravitational pressure drop and the frictional pressure drop remain constant, the contribution of the frictional pressure drop decreases. However, the previous increase of the Taylor bubble frictional pressure drop compensates this (note that the liquid slug frictional pressure drop is approximately double in absolute terms that of the Taylor bubble region).

Finally, the entrainment factor, \( FE \), is usually of minor importance in slug flow. In this model and this case, it barely affects the Taylor bubble liquid holdup, \( H_{TB} \), and thus the slug unit liquid holdup does not effectively change. It affects slightly more the pressure drop: as \( FE \) increases, more liquid goes through the small droplets inside the Taylor bubble region, and the film velocity, \( v_{LTB} \), decreases slightly. Due to a lower \( Ref \), the friction factor \( f_f \) increases slightly. The resulting effect is that the frictional pressure drop in the Taylor bubble decreases in absolute value, and the overall pressure drop, \( dp/dL \), increases. However, this augmentation is very small in comparison with the other sensitivity coefficients.

Table 3.3: Representative Kuwaiti well case study properties

<table>
<thead>
<tr>
<th>( d [\text{m}] )</th>
<th>( \rho_g [\text{kg/m}^3] )</th>
<th>( \rho_L [\text{kg/m}^3] )</th>
<th>( \mu_g [\text{Pa} \cdot \text{s}] )</th>
<th>( \mu_L [\text{Pa} \cdot \text{s}] )</th>
<th>( \sigma [\text{N/m}] )</th>
<th>( v_{SG} [\text{m/s}] )</th>
<th>( v_{SL} [\text{m/s}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1524</td>
<td>30</td>
<td>850</td>
<td>1.5 \times 10^{-5}</td>
<td>8 \times 10^{-3}</td>
<td>0.02</td>
<td>4.5</td>
<td>0.2</td>
</tr>
</tbody>
</table>

Furthermore, we analyze more cases that cover the fluid property ranges studied in more detail in chapter 6 and 7. In order to compare them, average normalized coefficients including the results of all of them are calculated. For each case study, \( j \), the absolute value of the
Table 3.4: Sensitivity coefficients for the representative Kuwaiti well case study

<table>
<thead>
<tr>
<th></th>
<th>$\phi_{f,i} (H_{SU})$</th>
<th>$\phi_{g,i} (dp/dL)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orell and Rembrand (1986)</td>
<td>$v_{TB}$ $H_{LS}$</td>
<td>$v_{TB}$ $H_{LS}$</td>
</tr>
<tr>
<td></td>
<td>2.78 1.41-10$^{-1}$</td>
<td>3.12 7.35-10$^{-2}$</td>
</tr>
<tr>
<td>Ansari et al. (1994)</td>
<td>$v_{TB}$ $H_{LS}$ $v_{gLS}$ $v_{LTB}$</td>
<td>$v_{TB}$ $H_{LS}$ $v_{gLS}$ $v_{LTB}$</td>
</tr>
<tr>
<td></td>
<td>1.69 1.20-10$^{-1}$ 1.38 -1.15-10$^{-12}$</td>
<td>1.09 -1.12-10$^{-1}$ 1.23 2.88-10$^{-1}$</td>
</tr>
<tr>
<td>Petalas and Aziz (2000)</td>
<td>$v_{TB}$ $H_{LS}$ $v_{gLS}$ $\beta$ $FE$</td>
<td>$v_{TB}$ $H_{LS}$ $v_{gLS}$ $\beta$ $FE$</td>
</tr>
<tr>
<td></td>
<td>1.78 -5.39-10$^{-3}$ 1.19 0 0</td>
<td>2.53 -3.41 2.08 1.50 3-10$^{-1}$</td>
</tr>
</tbody>
</table>

slug unit liquid holdup sensitivity coefficients with respect to the mechanistic model’s closure relations, $i$, $|\phi_{f,i,j}|$, are normalized by the maximum sensitivity coefficient of this case study $j$, $\max_{i} |\phi_{f,i,j}|$. The results are then averaged over the number of cases done, $n$. That is, the slug unit liquid holdup average normalized coefficient with respect to the closure relation $i$ is

$$\bar{c}_{f,i} = \frac{1}{n} \sum_{j=1}^{n} \frac{|\phi_{f,i,j}|}{\max_{i} |\phi_{f,i,j}|}. \quad (3.47)$$

The higher the value of $\bar{c}_{f,i}$, the more dominant the closure relation $i$ is on $H_{SU}$, the maximum being equal to one, $0 \leq \bar{c}_{f,i} \leq 1$. Similarly, the pressure drop average normalized coefficient with respect to the closure relation $i$ is

$$\bar{c}_{g,i} = \frac{1}{n} \sum_{j=1}^{n} \frac{|\phi_{g,i,j}|}{\max_{i} |\phi_{g,i,j}|}. \quad (3.48)$$

The cases and results for each model are shown in the following subsections.

### 3.4.1 Orell and Rembrand (1986)

Table 3.5 shows the cases studied with the model of Orell and Rembrand (1986). The average normalized coefficients $\bar{c}_{f,i}$ and $\bar{c}_{g,i}$ obtained are shown in table 3.6. Similar to the Kuwaiti well case study, the Taylor bubble velocity, $v_{TB}$, is dominant over the liquid slug
liquid holdup, $H_{LS}$, with respect to both the slug unit liquid holdup, $H_{SU}$, and the pressure drop, $dp/dL$. Furthermore, $\bar{c}_{g,v_{TB}} = 1$, which means that $v_{TB}$ affects the outcome of $dp/dL$ greater than $H_{LS}$ for all cases analyzed.

Table 3.5: Case studies for Orell and Rembrand (1986)

<table>
<thead>
<tr>
<th>$d$ [m]</th>
<th>$\rho_g$ [kg/m$^3$]</th>
<th>$\rho_L$ [kg/m$^3$]</th>
<th>$\mu_g$ [Pa·s]</th>
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<th>$\sigma$ [N/m]</th>
<th>$v_{SG}$ [m/s]</th>
<th>$v_{SL}$ [m/s]</th>
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<tr>
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<td>4</td>
<td>3</td>
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</table>

3.4.2 Ansari et al. (1994)

Table 3.7 shows the cases studied with the model of Ansari et al. (1994). The average normalized coefficients obtained are shown in table 3.8. Once again, results shown the same behavior as the Kuwaiti case: that $v_{TB}$ is dominant together with $v_{gLS}$ for both $dp/dL$ and $H_{SU}$.

72
Table 3.6: Sensitivity coefficients in Orell and Rembrand (1986) of cases from table 3.5

<table>
<thead>
<tr>
<th>$\tilde{c}<em>{f,i}$ ($H</em>{SU}$)</th>
<th>$\tilde{c}_{g,i}$ ($dp/dL$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$v_{TB}$</td>
<td>$H_{LS}$</td>
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<tr>
<td>9.72·10⁻¹</td>
<td>2.44·10⁻¹</td>
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</table>

3.4.3 Petalas and Aziz (2000)

Table 3.9 shows the cases studied with the model of Petalas and Aziz (2000). Since this mechanistic model is a unified one, seven different inclination angles are studied, from vertical to almost horizontal: $\theta = 90^\circ, 75^\circ, 60^\circ, 45^\circ, 30^\circ, 15^\circ$ and $5^\circ$. Cases shown in table 3.9 are intermittent flow regime for $\theta = 90^\circ$. For certain inclination angles, some of these cases are not intermittent flow based on the flow regime prediction model of Petalas and Aziz (2000), and are not included in the computation of the average normalized coefficients, whose values are shown in table 3.10. Again, results show that $v_{TB}$ is dominant together with $H_{LS}$ and $v_{gLS}$ for $dp/dL$, and $v_{gLS}$ for $H_{SU}$, similarly to the Kuwaiti case. It is interesting to note that the sensitivity of $H_{SU}$ with respect to $H_{LS}$ increases with decreasing inclination angle –although it is still around 20% that of $v_{TB}$ for its maximum at $\theta = 5^\circ$. 

73
Table 3.7: Case studies for Ansari et al. (1994)

<table>
<thead>
<tr>
<th>$d$ [m]</th>
<th>$\rho_g$ [kg/m$^3$]</th>
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</tbody>
</table>
Table 3.8: Sensitivity coefficients in Ansari et al. (1994) of cases from table 3.7

\[
\begin{array}{ccccccccc}
\bar{c}_{f,i} (H_{SU}) & | & \bar{c}_{g,i} (dp/dL) \\
\hline
v_{TB} & H_{LS} & v_{gLS} & v_{LTB} & v_{TB} & H_{LS} & v_{gLS} & v_{LTB} \\
9.82 \cdot 10^{-1} & 5.08 \cdot 10^{-2} & 8.11 \cdot 10^{-1} & 3.57 \cdot 10^{-2} & 7.57 \cdot 10^{-1} & 2.94 \cdot 10^{-1} & 9.98 \cdot 10^{-1} & 2.11 \cdot 10^{-1} \\
\end{array}
\]
Table 3.9: Case studies for Petalas and Aziz (2000)

<table>
<thead>
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<td>0.05</td>
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<td>3</td>
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<tr>
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<td>0.3</td>
<td>0.035</td>
<td>2</td>
<td>0.1</td>
</tr>
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</tr>
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<td>0.035</td>
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<td>0.035</td>
<td>2</td>
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</tr>
<tr>
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<td>0.000015</td>
<td>0.3</td>
<td>0.035</td>
<td>0.1</td>
<td>2</td>
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</tbody>
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76
Table 3.10: Sensitivity coefficients in Petalas and Aziz (2000) of cases from table 3.9

<table>
<thead>
<tr>
<th>$\theta$ [$^\circ$]</th>
<th>$v_{TB}$</th>
<th>$H_{LS}$</th>
<th>$v_{gLS}$</th>
<th>$\beta$</th>
<th>$FE$</th>
<th>$v_{TB}$</th>
<th>$H_{LS}$</th>
<th>$v_{gLS}$</th>
<th>$\beta$</th>
<th>$FE$</th>
</tr>
</thead>
<tbody>
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<td>90</td>
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<td>$3.15\times10^{-2}$</td>
<td>$6.92\times10^{-1}$</td>
<td>0</td>
<td>0</td>
<td>$5.69\times10^{-1}$</td>
<td>$5.46\times10^{-1}$</td>
<td>$5.90\times10^{-1}$</td>
<td>$2.82\times10^{-1}$</td>
<td>$1.49\times10^{-14}$</td>
</tr>
<tr>
<td>75</td>
<td>$7.88\times10^{-1}$</td>
<td>$3.79\times10^{-2}$</td>
<td>$6.90\times10^{-1}$</td>
<td>0</td>
<td>0</td>
<td>$5.74\times10^{-1}$</td>
<td>$5.09\times10^{-1}$</td>
<td>$6.10\times10^{-1}$</td>
<td>$3.02\times10^{-1}$</td>
<td>$2.06\times10^{-14}$</td>
</tr>
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<td>60</td>
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<td>$6.83\times10^{-2}$</td>
<td>$6.76\times10^{-1}$</td>
<td>0</td>
<td>0</td>
<td>$5.82\times10^{-1}$</td>
<td>$5.11\times10^{-1}$</td>
<td>$5.88\times10^{-1}$</td>
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<td>$1.76\times10^{-14}$</td>
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<td>$6.66\times10^{-1}$</td>
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<td>$5.15\times10^{-1}$</td>
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</tr>
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<td>$1.26\times10^{-1}$</td>
<td>$6.54\times10^{-1}$</td>
<td>0</td>
<td>0</td>
<td>$5.58\times10^{-1}$</td>
<td>$5.22\times10^{-1}$</td>
<td>$5.53\times10^{-1}$</td>
<td>$3.36\times10^{-1}$</td>
<td>$2.53\times10^{-14}$</td>
</tr>
<tr>
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<td>$1.38\times10^{-1}$</td>
<td>$6.44\times10^{-1}$</td>
<td>0</td>
<td>0</td>
<td>$5.16\times10^{-1}$</td>
<td>$5.76\times10^{-1}$</td>
<td>$5.24\times10^{-1}$</td>
<td>$3.53\times10^{-1}$</td>
<td>$3.94\times10^{-14}$</td>
</tr>
<tr>
<td>5</td>
<td>$8.04\times10^{-1}$</td>
<td>$1.60\times10^{-1}$</td>
<td>$6.11\times10^{-1}$</td>
<td>0</td>
<td>0</td>
<td>$5.28\times10^{-1}$</td>
<td>$5.79\times10^{-1}$</td>
<td>$5.25\times10^{-1}$</td>
<td>$3.70\times10^{-1}$</td>
<td>$1.70\times10^{-14}$</td>
</tr>
</tbody>
</table>
3.5 Conclusions

Based on the results of the sensitivity study, it is concluded that an improvement in the prediction of the Taylor bubble terminal velocity, $v_{TB}$, will have a higher impact in the mechanistic models than any other closure relation. Thus, the project is focused from now on the dynamics of Taylor bubbles in inclined pipes with both stagnant liquid and fluid flow.
4.1 Introduction

In this chapter, the multiphase CFD code used in our study is described and then validated against experimental data, correlations and models of the bubble terminal velocity, film thickness and shape. Numerical results are accurate enough to employ confidently the code as a tool to study further the Taylor bubbles in slug flow of vertical and inclined pipes with stagnant and flowing liquid.

4.2 CMFD code description

3-D CMFD simulations have been performed with the CMFD code TransAT® (2014), a finite-volume software developed at ASCOMP. The code uses structured meshes and MPI parallel-based algorithm to solve multi-fluid Navier-Stokes equations. Computer resources for this work include the supercomputers Titan and Eos of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, where around two million core hours were used.
TransAT® (2014) uses the one-fluid formulation approach, where the flow is described by one fluid with variable material properties, which vary according to a color function, which is advected by the flow, thus identifying the gas and liquid regions. In the absence of phase change phenomena, the mass and momentum conservation equations are

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{4.1a}
\]

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \bar{\sigma} + \rho \mathbf{g} + \mathbf{F}_s, \tag{4.1b}
\]

where \( t \) is the time, \( \mathbf{v} \) is the velocity vector, \( p \) is the pressure, \( \bar{\sigma} = \mu(\nabla \mathbf{v} + (\nabla \mathbf{v})^T) \) is the viscous stress tensor, and \( \mathbf{F}_s = \sigma \kappa \mathbf{n} \delta(\phi) \) is the surface tension term where \( \kappa = -\nabla \phi/|\nabla \phi| \) is the surface curvature, \( \mathbf{n} \) is the vector normal to the interface, and \( \delta \) is a smoothed delta function centered at the interface. In this work, the color function used is based on the Level Set (LS) method (Osher and Sethian, 1988), where the interface is represented by a continuous and monotonous function \( \phi \) that represents the distance to the interface at which \( \phi = 0 \). The LS advection equation is given by

\[
\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla \phi = 0, \tag{4.2}
\]

and material properties such as density and viscosity are updated locally based on \( \phi \), and smoothed across the interface using a smooth Heaviside function. A mass conservation scheme is also employed to avoid scheme-induced losses. Furthermore, the pipe is modeled as an embedded surface and represented in the fluid by the so-called Solid Level Set function where \( \phi_s = 0 \) is the fluid-solid interface, i.e. the Immersed Surfaces Technology (IST) technique (Chung, 2001; Labois et al., 2010). This method is a variant of the Immersed Boundary Method (Peskin, 1977; Mittal and Iaccarino, 2005). The no-slip condition at the wall is imposed through a relaxation term which acts as a distributed momentum sink reducing the fluid velocity as the indicator function goes to zero (Beckermann et al., 1999).

The mesh is locally refined next to the pipe walls. Then, the meshed domain is decomposed into a number of blocks equal to the number of processors used for the calculation.
Transfer of information between neighboring blocks is performed using MPI parallelization. Simulations are carried out using the 2nd-order Hybrid Linear/Parabolic Approximation (HLPA) scheme (Zhu, 1991) for the discretization of the convective fluxes, which combines a 2nd-order upstream-weighted approximation with 1st-order upwind differencing under the control of a convective boundedness criterion, and is a compromise between the large numerical diffusion of the 1st-order upwind schemes and the numerical instability problem for the higher order upwind schemes with low numerical diffusion. An implicit 1st-order scheme is used for the time marching, where the time-step is adaptive and bounded by a Courant number fixed between 0.5 and 0.9 to guarantee stability of the simulations. The SIMPLEC (Semi-Implicit Method for Pressure Linked Equations-Consistent) algorithm is used for the pressure-velocity coupling (Doormaal and Raithby, 1984). Finally, the solvers used depend on the simulation. For high viscosity cases where the Navier-Stokes equations tend to elliptic, the R-cycle adaptive Algebraic Multigrid (AMG) method is used (R-cycle, 2016). Otherwise, either the incomplete lower-upper decomposition method Strongly Implicit Procedure (SIP) (Stone, 1968) or the Generalized Minimum Residual method (GMRES) (Saad and Schultz, 1986) are used, the latter with hypre AMG preconditioning (Falgout et al., 2006) of the parallel PETSc (Portable, Extensible Toolkit for Scientific Computation) library (Balay et al., 1997).

Before conducting the DNS simulations, the discretization schemes are evaluated with the following test case: a 2D vortex is convected by a uniform flow on a periodic 3D mesh. After a certain convective time, supposing that there are no interactions between the various vortices on the infinite domain, the vortex profile should be the same as the initial one. The test is illustrated in figure 4-1a. The fluid is considered to be non-viscous and no turbulence model is used. Thus, the only source of dissipation comes from the numerical schemes. The numerical error introduced by the discretization schemes can be estimated by the \(l^2\)–norm of the difference between the initial and final velocity profiles at \(t = t_{\text{initial}}\) and \(t = t_{\text{final}}\), respectively:

\[
l^2 = \sqrt{\sum_{\text{cells}} |v_{\text{final}} - v_{\text{initial}}|^2 / \sum_{\text{cells}} |v_{\text{initial}}|^2}
\]  

(4.3)
The spacial convergence, shown in figure 4-1b, is satisfactory.

In this work, we perform two main types of simulations: a Taylor bubble in a closed pipe (section 4.3 below, and chapter 6), and Taylor bubble in a pipe with liquid flow (chapter 7). In the first type, the simulations start with a single bubble in still liquid and finish when the bubble reaches its terminal velocity. The bubble is placed inside a closed pipe embedded in the numerical domain (see figure 4-2). The boundary conditions of the numerical domain are symmetry planes where the normal velocity and pressure gradient components are set to zero. The solid phase velocity is set to zero, and the no-slip condition at the wall is imposed through a relaxation term which acts as a distributed momentum sink reducing the fluid velocity as the indicator function goes to zero (Beckermann et al., 1999). The structured mesh size is dependent on the case study and is refined until the terminal velocity converges (see figure 4-3). The mesh is locally refined next to the pipe walls. Number of cells ranges from 1 million up to 5 million cells.

For Taylor bubbles in pipes with liquid flow, the simulations start with a single bubble in still liquid and finish when the bubble reaches its terminal velocity, similar to the simulations of bubbles in stagnant liquid. The bubble is placed inside a pipe with both ends open and embedded in the numerical domain. The boundary conditions of the numerical domain are
Figure 4-2: Snapshot of the computational domain for the simulations of chapter 6

Figure 4-3: Mesh convergence for case 1 of table 4.2
an inflow plane at the pipe inlet where the velocity is set to a transient profile that evolves from zero at the simulation start to the Hagen-Poiseuille profile, an outflow plane at the pipe outlet where the stream-wise gradients of all variables are set to zero (fully developed flow condition) and overall mass conservation is ensured, and finally symmetry planes at the other four planes parallel to the pipe longitudinal axis where the normal velocity and pressure gradient components are set to zero. The no-slip condition at the wall is imposed as the simulations of bubbles in stagnant liquid, and the structured mesh size is also dependent on the case study and is refined until the terminal velocity converges. In this type, number of cells ranges from 1 million up to 3.7 million cells.

4.3 Code validation

4.3.1 Vertical pipes

Table 4.2 shows the test matrix for simulations of Taylor bubble motion in vertical pipes \((\theta = 90^\circ)\) with no imposed flow \((Re = 0)\) performed with TransAT® (2014), whose cases are localized in the experimental map of White and Beardmore (1962) in figure 4-4, where the \(x\)-axis is the \(Eo\) number, and the \(y\)-axis is the \(Mo\) number.

The numerically obtained \(Fr\) number is successfully compared to its values found in the literature. Six cases are compared with experimental data (cases 3 and 4 with Shosho and Ryan (2001); case 5 with Bugg and Saad (2002); case 7 with Nogueira et al. (2006); case 8 with Jeyachandra et al. (2012); and case 10 with Tomiyama et al. (2001)), whereas the other four cases are compared with the correlation of Viana et al. (2003). The average terminal velocity error of the simulations is \(-1.4\%\), with a standard deviation equal to 10.4\%. Using the correlation of Viana et al. (2003) for cases 3 and 4 instead of the experimental values of Shosho and Ryan (2001), the error is \(0.182 \pm 6.1\%\). Figure 4-5 shows a graphical comparison between the numerical and the literature \(Fr\) values of table 4.2. Similarly, the developed non-dimensional film thickness \(\bar{h} = h/d\), where \(d\) is the pipe diameter, compares well with data from the literature. Two cases are compared with experimental data (case
Table 4.1: Test matrix for simulations of Taylor bubble motion in vertical pipes ($\theta = 90^\circ$) with no imposed flow ($Re = 0$)

<table>
<thead>
<tr>
<th>Case</th>
<th>Mo</th>
<th>$Eo$</th>
<th>$N_f$</th>
<th>$Fr$ (lit)</th>
<th>$Fr$ (sim)</th>
<th>$\bar{h}$ (lit)</th>
<th>$\bar{h}$ (sim)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.328</td>
<td>76.5</td>
<td>34.2</td>
<td>0.210</td>
<td>0.212</td>
<td>0.148</td>
<td>0.144</td>
</tr>
<tr>
<td>2</td>
<td>4.03$\cdot 10^{-3}$</td>
<td>187</td>
<td>201</td>
<td>0.324</td>
<td>0.306</td>
<td>0.099</td>
<td>0.094</td>
</tr>
<tr>
<td>3</td>
<td>19.2</td>
<td>31.2</td>
<td>6.31</td>
<td>0.0573</td>
<td>0.0418</td>
<td>0.153</td>
<td>0.146</td>
</tr>
<tr>
<td>4</td>
<td>1.17$\cdot 10^{-4}$</td>
<td>38.6</td>
<td>149</td>
<td>0.276</td>
<td>0.295</td>
<td>0.106</td>
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</tr>
<tr>
<td>5</td>
<td>1.52$\cdot 10^{-2}$</td>
<td>98.4</td>
<td>89.0</td>
<td>0.303</td>
<td>0.291</td>
<td>0.123</td>
<td>0.119</td>
</tr>
<tr>
<td>6</td>
<td>1.50$\cdot 10^{-3}$</td>
<td>9.88</td>
<td>28.3</td>
<td>0.0411</td>
<td>0.0458</td>
<td>0.096</td>
<td>0.094</td>
</tr>
<tr>
<td>7</td>
<td>4.75$\cdot 10^{-2}$</td>
<td>192</td>
<td>111</td>
<td>0.336</td>
<td>0.322</td>
<td>0.117</td>
<td>0.109</td>
</tr>
<tr>
<td>8</td>
<td>8.38</td>
<td>747</td>
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<td>0.130</td>
</tr>
<tr>
<td>9</td>
<td>8.38</td>
<td>181</td>
<td>29.0</td>
<td>0.199</td>
<td>0.216</td>
<td>0.153</td>
<td>0.148</td>
</tr>
<tr>
<td>10</td>
<td>3.73$\cdot 10^{-11}$</td>
<td>23.8</td>
<td>4,360</td>
<td>0.300</td>
<td>0.285</td>
<td>0.036</td>
<td>0.051</td>
</tr>
</tbody>
</table>

5 (Bugg and Saad, 2002); and case 7 (Nogueira et al., 2006)). The other eight cases are compared with the correlations provided by Llewellin et al. (2012): their so-called Cubic Brown model (equations 2.5 and 2.6 in their article) for cases where the flow in the film is laminar ($N_f \leq 1372$), and an empirical correlation (equation 4.2 in their article) for case 10, where $N_f > 1,372$. The Fr needed for these correlations are obtained from the expression of Viana et al. (2003). The average film thickness error of the simulations is $0.457 \pm 6.26\%$.

Figure 4-5 shows a graphical comparison between the numerical and the literature $\bar{h}$ values of table 4.2.

TransAT® code has been validated using data from the literature for the Taylor bubble terminal velocity in inclined pipes and in vertical pipes. The calculated bubble shape is compared with experimental data from Nogueira et al. (2006) for case 7 (figure 4-6), and the calculated velocity vectors are compared to experimental Particle Image Velocimetry (PIV) data from Bugg and Saad (2002)$^1$ for case 5 (figure 4-7 to figure 4-9).

In figure 4-6, the bubble profile in the $yz$-plane (where the $z$-axis is the vertical) overlaps with the bubble profile in the perpendicular $xz$-plane, confirming an axisymmetric profile.

$^1$Note that error bars are not available
Figure 4-4: The map of White and Beardmore (1962) with the location of the numbered cases to validate the CMFD code: circles (○) indicate the cases of table 4.2, and the squares (□) indicate the experimental cases performed in our laboratory.

Figure 4-5: Taylor bubble terminal $Fr$ (a) and dimensionless film thickness, $\tilde{h}$, (b) numerical results compared with the values obtained from literature correlations for vertical pipes.
Figure 4-7s shows the axial velocity component along the tube axis above the tip of the bubble: note that the presence of the bubble does not affect the flow beyond one diameter ahead of its tip. The axial and radial velocity components at $z/R = 0.222$ above the bubble tip are shown on figure 4-7b. The axial velocity is positive in the center region of the pipe, and becomes negative in the periphery due to the suction of the film around the Taylor bubble. The radial velocity is zero at the tube axis due to symmetry and at $z/R = 1$ due to the tube wall, and is positive elsewhere since liquid is moving from the center region towards the pipe wall where it is suctioned by the liquid film. Figure 4-8a shows the axial and radial velocity components in the film transition region at $z/R = 1.008$ below the bubble nose. The film is still developing since the radial velocity is not zero there. The axial velocity is negative in the whole film region. PIV particles are only observed in the liquid region, and the absence of them indicates the presence of the gas phase. Figure 4-8b shows the axial velocity profile in the fully developed falling film at a distance $z/R = 4.64$ from the bubble nose. In this fully developed region, the radial velocity is zero as expected. Finally, Figure 4-9 depicts the axial and radial velocity components in the wake of the bubble at a distance $z/R = 0.4$ below the bubble tail. The radial velocity is negative since the liquid coming from the falling film at the pipe wall moves towards the pipe inner core. Furthermore, the axial velocity is positive in the inner core, and negative in the outer core due to the falling film, a characteristic of the recirculation taking place in this case’s bubble wake. The comparison between simulations and experiments is successful and provides confidence in the use of TransAT® in this study.

### 4.3.2 Inclined pipes

3D CFD simulations of inclined pipes have been performed for cases 1, 3, 4, 8 and 9 from table 4.2. Figure 4-10 compares the $Fr$ number obtained numerically is compared with the experimental data of Shosho and Ryan (2001), and the correlations from Bendiksen (1984), Weber et al. (1986), Hasan and Kabir (1988a), Petalas and Aziz (2000), Gokcal et al. (2009b), Jeyachandra et al. (2012), Moreiras et al. (2014) (see section 6.2 of chapter 87.
Figure 4-6: The Taylor bubble shape of case 7 obtained numerically is compared with the experimental results from Nogueira et al. (2006).

Figure 4-7: The velocity profile of case 5 ahead of the bubble in the pipe centerline (a) and across the radial axis (b) obtained numerically is compared with the experimental data of Bugg and Saad (2002).
Figure 4-8: The velocity profile of case 5 in the developing region of the falling film (a) and in the developed film (b) obtained numerically is compared with the experimental data of Bugg and Saad (2002).

Figure 4-9: The velocity profile of case 5 in the wake of the bubble along the radial axis obtained numerically is compared with the experimental data of Bugg and Saad (2002).
Figure 4-10: $Fr$ as a function of $\theta$ for cases 3 (a) and 4 (b) compared with experiments from Shosho and Ryan (2001), and experimental correlations from the literature.

Numerical results compare well with the experimental data. Terminal velocity increases as the pipe inclines. The maximum value results from the competing effects of drag coefficient (lower at lower angles, where most of the liquid “bypasses” the bubble through a larger flow area), and buoyancy (higher at higher angle). Furthermore, successful simulations have been performed down to an inclination angle of 3 degrees for case 4 (figure 4-10b), where a thin film persists between the bubble and the wall and lubricates the bubble motion. As the inclination angle approaches zero, the bubble terminal velocity drops significantly showing a trend towards zero. Among the correlations used, the one from Hasan and Kabir (1988a) captures relatively well the trend of terminal velocity with inclination angle, where the maximum occurs close to the experimental and numerical values in the five cases. However, we think there is room for improvement in the value prediction.

Furthermore, the experiments described later in section 5.3.1, chapter 5, are also used to validate the model. Experiments and simulations of Taylor bubbles in an inclined pipe with stagnant mixtures of 50% DI water and 50% methanol ($Eo = 47$, $Mo = 3.8 \cdot 10^{-9}$, $N_f = 2,200$) and 25% DI water and 75% methanol ($Eo = 57$, $Mo = 3.1 \cdot 10^{-9}$, $N_f = 2,800$) are performed. The Taylor bubble terminal $Fr$ of these mixtures with respect to the inclination
angle is shown in figure 4-11, where $\theta = 90^\circ$ is the vertical. Tables 4.2 and 4.3 show the results. All cases behave well, where the case of $\theta = 5^\circ$ reports the worse comparison with an error of 6.62% for the 50%-50% mixture, and the case of $\theta = 30^\circ$ reports the worse comparison with an error of -6.82% for the 25%-75% mixture.

Furthermore, the experimental tip bubble shape of two different volumes is compared with the one obtained in simulations. Figures 4-12 to 4-16 depict the shape comparison for $\theta = 45^\circ$, 37.5°, 30°, 15°, and 5°, respectively. Bubble volume $V_1$ is characterized by $\lambda = 3.5$, where parameter $\lambda$ is calculated as $\lambda = d_e/d$, where $d_e$ is the sphere-volume equivalent diameter of the bubble. Bubble volume $V_2$ is characterized by $\lambda = 2.3$ for $\theta = 45^\circ$, $\lambda = 2.2$ for $\theta = 37.5^\circ$, $5^\circ$, and $\lambda = 2.4$ for $\theta = 30^\circ$, 15°. Finally, the simulated bubble volumes are characterized by $\lambda = 1.4$ for $\theta = 45^\circ$, 37.5°, $\lambda = 1.3$ for $\theta = 30^\circ$, 15°, and $\lambda = 1.2$ for $\theta = 5^\circ$. It can be seen that tip bubble shapes perfectly overlap.

Figure 4-11: Experimental and numerical values of $Fr$ as a function of $\theta$ for the mixture of 50% DI water and 50% methanol ($E_o = 47$, $Mo = 3.8 \cdot 10^{-9}$, $N_f = 2,200$) (a) and the mixture of 25% DI water and 75% methanol ($E_o = 57$, $Mo = 3.1 \cdot 10^{-9}$, $N_f = 2,800$) (b) compared with experimental correlations from the literature.
Table 4.2: Experimental and numerical Fr for the mixture of 50% DI water and 50% methanol ($Eo = 47, Mo = 3.8 \cdot 10^{-9}, N_f = 2,200$)

<table>
<thead>
<tr>
<th>$\theta$ [$^\circ$]</th>
<th>Fr (Experiments)</th>
<th>Fr (Viana et al., 2003)</th>
<th>Fr (Simulations)</th>
<th>Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>90</td>
<td>-</td>
<td>0.3338</td>
<td>0.3335</td>
<td>0.08</td>
</tr>
<tr>
<td>45</td>
<td>0.4416</td>
<td>-</td>
<td>0.4295</td>
<td>-2.75</td>
</tr>
<tr>
<td>37.5</td>
<td>0.4464</td>
<td>-</td>
<td>0.4407</td>
<td>-1.27</td>
</tr>
<tr>
<td>30</td>
<td>0.4393</td>
<td>-</td>
<td>0.4268</td>
<td>-2.83</td>
</tr>
<tr>
<td>15</td>
<td>0.4115</td>
<td>-</td>
<td>0.4086</td>
<td>-0.70</td>
</tr>
<tr>
<td>5</td>
<td>0.3638</td>
<td>-</td>
<td>0.3878</td>
<td>6.62</td>
</tr>
</tbody>
</table>

Table 4.3: Experimental and numerical Fr for the mixture of 25% DI water and 75% methanol ($Eo = 57, Mo = 3.1 \cdot 10^{-9}, N_f = 2,800$)

<table>
<thead>
<tr>
<th>$\theta$ [$^\circ$]</th>
<th>Fr (Experiments)</th>
<th>Fr (Simulations)</th>
<th>Error [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>90</td>
<td>0.3365</td>
<td>0.3340</td>
<td>-0.72</td>
</tr>
<tr>
<td>75</td>
<td>0.3890</td>
<td>0.3757</td>
<td>-3.41</td>
</tr>
<tr>
<td>60</td>
<td>0.4173</td>
<td>0.4166</td>
<td>-0.16</td>
</tr>
<tr>
<td>45</td>
<td>0.4504</td>
<td>0.4460</td>
<td>-0.98</td>
</tr>
<tr>
<td>37.5</td>
<td>0.4598</td>
<td>0.4481</td>
<td>-2.53</td>
</tr>
<tr>
<td>30</td>
<td>0.4597</td>
<td>0.4284</td>
<td>-6.82</td>
</tr>
<tr>
<td>15</td>
<td>0.4243</td>
<td>0.4075</td>
<td>-3.97</td>
</tr>
<tr>
<td>5</td>
<td>0.3828</td>
<td>0.3891</td>
<td>1.65</td>
</tr>
</tbody>
</table>
Figure 4-12: Tip bubble shape comparison between experimental and numerical results for the mixture of 50\% DI water and 50\% methanol in volume and $\theta = 45^\circ$ for two different bubble volumes, $V_1$ ($\lambda = 3.5$) (a) and $V_2$ ($\lambda = 2.3$) (b), where $\lambda = 1.4$ for the simulated bubble.

Figure 4-13: Tip bubble shape comparison between experimental and numerical results for the mixture of 50\% DI water and 50\% methanol in volume and $\theta = 37.5^\circ$ for two different bubble volumes, $V_1$ ($\lambda = 3.5$) (a) and $V_2$ ($\lambda = 2.2$) (b), where $\lambda = 1.4$ for the simulated bubble.
Figure 4-14: Tip bubble shape comparison between experimental and numerical results for the mixture of 50% DI water and 50% methanol in volume and $\theta = 30^\circ$ for two different bubble volumes, $V_1 (\lambda = 3.5)$ (a) and $V_2 (\lambda = 2.4)$ (b), where $\lambda = 1.3$ for the simulated bubble.

Figure 4-15: Tip bubble shape comparison between experimental and numerical results for the mixture of 50% DI water and 50% methanol in volume and $\theta = 15^\circ$ for two different bubble volumes, $V_1 (\lambda = 3.5)$ (a) and $V_2 (\lambda = 2.4)$ (b), where $\lambda = 1.3$ for the simulated bubble.
Figure 4-16: Tip bubble shape comparison between experimental and numerical results for the mixture of 50% DI water and 50% methanol in volume and $\theta = 5^\circ$ for two different bubble volumes, $V_1$ ($\lambda = 3.5$) (a) and $V_2$ ($\lambda = 2.2$) (b), where $\lambda = 1.2$ for the simulated bubble.
Figure 4-17: Tip bubble shape comparison between experimental and numerical results for the mixture of 25% DI water and 75% methanol in volume and eight different inclination angles
4.4 Conclusions

In this chapter, the CFD code TransAT® is described and then validated against experimental data, correlations and models of the bubble terminal velocity, film thickness and shape. Numerical results were accurate enough to employ confidently the code as a tool to study further the Taylor bubbles in slug flow of vertical and inclined pipes with stagnant and flowing liquid.
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Chapter 5

Justification of Key Assumptions Made in the Simulations

5.1 Introduction

In this chapter, the two main assumptions used in the simulations of the study are presented and analyzed. First, it is assumed that the lubricating liquid film formed above the bubble as the pipe inclines with respect to the horizontal does not breakup. That is, the gas phase never touches the pipe and triple line is not formed. To verify the robustness of this assumption, the gravity-induced film drainage is analytically modeled and experimentally validated. From it a criterion to avoid film breakup is obtained, which holds in the simulations performed. Secondly, it is also assumed that the Taylor bubble length does not affect its dynamics in inclined pipes. This assumption is validated with both experiments and simulations.
5.2 Analytical film drainage model and breakup criterion

5.2.1 Problem description

In slug flow of vertical pipes, an axisymmetric lubricating film with a constant thickness surrounds the Taylor bubble. For stagnant liquid, the range of the non-dimensional film thickness, $\tilde{h} = h/R$, where $h$ is the film thickness and $R$ is the pipe radius, is approximately $\tilde{h} \in [0.08, 0.33]$ (see Llewellin et al., 2012). As the pipe inclination increases, the Taylor bubble approaches the pipe wall and the lubricating film becomes significantly thinner and non-axisymmetric; moreover, the thickness of the film decreases along the Taylor bubble due to azimuthal gravity-driven drainage. If the film breaks up, the surface tension force at the triple contact line reduces the velocity of the bubble significantly (Behafarid et al., 2015). Here, a simplified analysis proves that both situations (see figure 5-1) are dynamically different.

\[ \text{Figure 5-1: Schematic of the Taylor bubble with a lubricating thin film above it (a), and without it (b)} \]

In the analysis, it is assumed that the gas pressure, $p_g$, the liquid pressure at the nose,
and the tip radius, \( R_{tip} \), are all the same for both cases,

\[
P_{nose,a} \sim P_{nose,b} \sim P_{nose}, \quad (5.1a)
\]
\[
p_{g,a} \sim p_{g,b} \sim p_{g}, \quad (5.1b)
\]
\[
R_{tip,a} \sim R_{tip,b} \sim R_{tip}. \quad (5.1c)
\]

The pressures at the nose, \( P_{nose} \), at the liquid film, \( p_{film} \), and at the bubble gas, \( p_{g} \), can be related through the Young-Laplace equation (Langewisch, 2014),

\[
p_{g} - P_{nose} = \frac{2\sigma}{R}, \quad (5.2a)
\]
\[
p_{g} - p_{film} = \frac{\sigma}{R}, \quad (5.2b)
\]

where \( \sigma \) is the surface tension. When the thin film no longer exists, a triple line is formed and new capillary forces act on the bubble (see forces \( F_1 \) and \( F_2 \) in figure 5-1b). The components of the capillary force, \( F_x \) and \( F_y \), are calculated through circulation integrals,

\[
F_x = -\int_{l} \sigma \cos \theta(l)dl, \quad (5.3a)
\]
\[
F_y = \int_{l} \sigma \sin \theta(l)dl, \quad (5.3b)
\]

where the angle \( \theta(l) \) is a function of \( l \). If we subtract the \( x \) axis forces acting on the bubble for both cases, a net force dragging the bubble back against its movement up through the pipe results,

\[
F_{x,b} - F_{x,a} = -\int_{l} \sigma \cos \theta(l)dl. \quad (5.4)
\]

The dynamics in the \( y \) direction are more complex to analyze. It is assumed that the order of magnitude of the bubble cross sectional area perpendicular to the \( y \) axis, \( A_y \), is the same for both cases. Thus, the force component in case (a) is

\[
F_{y,a} = (p_{film} - p_{g}) A_y, \quad (5.5)
\]
whereas $F_{y,b}$ in case (b) is

$$F_{y,b} = \int_{l} \sigma \sin \theta(l) dl - p_g A_y. \quad (5.6)$$

Subtracting the previous equations 5.5 and 5.6, the following expression is obtained

$$F_{y,b} - F_{y,a} = \left( \int_{l} \sigma \sin \theta(l) dl - p_g A_y \right) - \left( p_{film} - p_g \right) A_y = \int_{l} \sigma \sin \theta(l) dl - p_{film} A_y. \quad (5.7)$$

The pressures at the film, $p_{film}$, and at the nose, $p_{nose}$, can be related through equations 5.2,

$$p_{film} - p_{nose} = \frac{\sigma}{R}, \quad (5.8)$$

thus

$$F_{y,b} - F_{y,a} = \int_{l} \sigma \sin \theta(l) dl - \left( \frac{\sigma}{R} + p_{nose} \right) A_y. \quad (5.9)$$

Equations 5.4 and 5.9 show that both systems are dynamically not equivalent, thus the importance to determine the physical reality.

### 5.2.2 Film drainage and breakup: literature review

The existence of this lubricating film and its breakup have received some attention in the nuclear and oil and gas industries. Maneri and Zuber (1974) and Hien and Fabre (2004a) studied the velocity of plane bubbles in two-dimensional ducts experimentally and numerically, respectively, using deionized (DI) water and methanol. They observed three different bubble shape regimes depending on the duct inclination: (i) the bubble touching the upper wall for $\theta \leq 60^\circ$, (ii) a stable lubricating film where the bubble does not touch the duct for $\theta > 80^\circ$, and (iii) an unstable transition region in between. Al-Safran et al. (2013) observed a stable thin film at the top of the horizontal pipe in their slug flow experiments with high-viscosity fluids. However, these results are valid for the limited set of fluid properties and flow conditions explored in those studies. The drainage of a vertical film due to gravity was analyzed by Mysels et al. (1959); here we extend the analysis to the situation where the component of gravity in the direction of the flow varies continuously, and surface tension
and intermolecular forces may affect the dynamics (Oron et al., 1997).

On the other hand, thin film between a particle and a bubble has been widely analyzed in the context of flotation (Nguyen and Schulze, 2003; Coons et al., 2003; Manev and Nguyen, 2005; Albijanic et al., 2010). There, the film thickness is on the order of nanometers and long-range intermolecular forces appear. In these cases, the interfacial stress balance is described by the so-called Augmented Young-Laplace Equation,

\[ p_g - p_L = p_\sigma - \Pi, \]

(5.10)

where the pressure difference across the interface, \( p_g - p_L \), is calculated using two terms: the capillary pressure, \( p_\sigma \),

\[ p_\sigma = \sigma \kappa, \]

(5.11)

where \( \kappa \) is the interface curvature which can be expressed in terms of the film thickness, \( h \), as

\[ \kappa = \frac{h''}{(1 + h'^2)^{3/2}}, \]

(5.12)

and, secondly, the disjoining pressure, \( \Pi \), where the long-range intermolecular force are captured. Although a detailed description of the forces involved in the disjoining pressure is beyond the scope of this work, a brief introduction is given here. The disjoining pressure was introduced by B. V. Derjaguin in the early 1930s (Derjaguin and Obuchov, 1935) to adequately expressed the deviations in the properties of the thin film from those of the bulk liquid phase. The thin liquid film is a phase of small thickness, in which the two interfacial layers overlap to form a unified non-homogeneous structure of specific properties (Manev and Nguyen, 2005). The disjoining pressure is a fundamental element in the classical Derjaguin-Landau-Verwey-Overbeek (DLVO) theory that incorporates the van-der-Waals and electrostatic double-layer interactions, \( \Pi = \Pi_{vdW} + \Pi_{elec} \), respectively. The van-der-Waals interaction can be expressed as a function of the film thickness \( h \) as

\[ \Pi_{vdW} = \frac{A(h, T, \kappa)}{6\pi h^3}, \]

(5.13)
where $A(h, T, \kappa^*)$ is the so-called Hamaker-Lifshitz constant which is a function of temperature $T$, the Debye constant $\kappa^*$, and weakly the film thickness $h$ (Manev and Nguyen, 2005). In foam and emulsion films the van-der-Walls disjoining pressure always attracts the film surfaces, i.e., $\Pi_{vdW}(A)$ is always negative. In asymmetrical films such as wetting films, $\Pi_{vdW}(A)$ can become positive when the liquid does not wet the surface. Furthermore, the electrostatic disjoining pressure $\Pi_{elec}$ arises in thin films from dilute electrolyte solutions and is due to the overlapping of the diffuse electric layers on the two film surfaces at small separation distances.

Film breakup occurs at this scale, where intermolecular forces act. Thus, particular attention has received its drainage in the literature. In the book of colloidal science of flotation (Nguyen and Schulze, 2003) the thinning and rupture of intervening liquid films are widely described. The thinning of liquid films between parallel planar surfaces is described by the Stefan-Reynolds equation (Stefan, 1874; Reynolds, 1886). When the driving forces are the capillary pressure and the forces included in the DLVO theory, the Stefan-Reynolds differential equation takes the form

$$\frac{dh}{dt} = -\frac{2h^3}{2\mu R^2}(p_\sigma - \Pi),$$

(5.14)

where $t$ is time, $\mu$ is the liquid viscosity, and $R$ is the film radius. The thinning differential equation of liquid films with deformed gas-liquid interfaces is

$$\frac{\partial h}{\partial t} = \frac{m}{12\tau \mu \partial r} \left( h^3, \frac{\partial p}{\partial r} \right),$$

(5.15)

where $m = 1 (4)$ for bubbles with an immobile (mobile) surface, and the pressure $p$ depends on the deformation of the gas-liquid interface and depends on $h$ (Nguyen and Schulze, 2003). Albijanic et al. (2010) reviewed the induction and attachment times of wetting thin films between air bubbles and particles. The equations are solved numerically (Li et al., 1990; Manica et al., 2008).

The rupture of wetting films on solid surfaces, our case, is an important step in a lot of
coagulation processes in colloidal systems. In particular, the forming, thinning and rupture of thin intervening water films play a crucial role in the interaction of an air bubble with a solid particle in the industrial flotation process (Schulze, 1984; Nguyen and Schulze, 2003), which is widely used in mineral processing, in paper recycling and waste water treatment. Two rupture mechanisms take place (Schulze et al., 2001; Stöckelhuber, 2003): (i) nucleation, and (ii) capillary wave mechanism or spinoidal dewetting.

The nucleation mechanism has been controversial for some years: there are cases where, although all DLVO-forces remain repulsive, the wetting film becomes unstable and ruptures. In this situation, the rupture thickness, also known as critical thickness, \( h_c \), can reach very high values and scatters strongly (Stöckelhuber, 2003). To explain this problem, some groups introduced a “long range hydrophobic force” of unknown physical origin (Israelachvili and Pashley, 1982, 1984). Now, it is widely accepted that the rupture of these films is a nucleation process due to the presence of nanobubbles on a hydrophobic solid surface (Ishida et al., 2000; Tyrrell and Attard, 2001; Ishida et al., 2002; Tyrrell and Attard, 2002; Lou et al., 2002; Stöckelhuber, 2003; Stöckelhuber et al., 2004). The mechanism here is similar to the film rupture in foam films, which has been extensively studied (Debrégeas et al., 1998; Bird et al., 2010).

Secondly, the capillary wave mechanism is based on classic hydrodynamic stability of the forces involved in the DLVO theory. Sheludko (1967) derived the condition for kinetic instability of the film based on the surface wave phenomenon, where a local concavity is developed due thermal fluctuations on the film surfaces. The capillary force acting in the locality of a fluctuation tries to heal the concavity, but a force cause by the disjoining pressure when attractive, tends to deepen it further. In the case of van-der-Waals attraction acting alone, as is the current study, the critical thickness, \( h_c \), is equal to

\[
h_c = \left( \frac{A\lambda_c^2}{128\sigma} \right)^{1/4},
\]

where \( \lambda_c \) is the critical wavelength. According to Scheludko the waves are limited by the film size and must be proportional to its radius. The optimal \( \lambda_c \) was estimated to be on the
order of $\lambda_c \sim 0.1R$, where $R$ is the radius of the circular thin film. Vrij (1966) obtained $\lambda_c$ in an explicit form, and derived two limiting expressions for the critical thickness, $h_c$, for negligible disjoining pressure with respect to the capillary pressure, and vice versa:

$$h_c = 0.222 \left( \frac{A r^2}{\sigma f} \right)^{1/4}, \quad \text{for} \quad \Pi \ll P_\sigma, \quad (5.17a)$$

$$h_c = 0.268 \left( \frac{A^2 r^2}{\sigma f} \right)^{1/7}, \quad \text{for} \quad \Pi \gg P_\sigma, \quad (5.17b)$$

where $f$ is a function of the initial thickness, $h_0$, and $\sigma$, but whose dependence on $h_0$ has been neglected. For example, $f$ ranges from 4.5 to 6.9 for $h_0 = 10$ to 100nm, using $\sigma = 0.03$N/m (Vrij, 1966).

The order of magnitude of wetting film critical thicknesses reported in the literature ranges from 1 to 100nm. Albijanic et al. (2010) reviewed the studies on critical rupture thickness of thin water film on hydrophobic surfaces, such as methylated fused-silica and mica plates, and it lied between 50 and 150nm. Stöckelhuber et al. (2004) reported a rupture film thicknesses in the interval of 20 to 100nm for pure water film, being films with surfactants in the upper bound. The most investigated systems in this field, aqueous wetting films on oxidized silica surfaces (i.e. quartz, glass or the oxide layer on silicon wafers), show a range from 13 to 60nm, depending on the electrolyte concentration in the water film (Stöckelhuber, 2003). Similar range of values are reported by Schulze et al. (2001), where the influence of the acting forces on the rupture mechanism (nucleation and capillary waves). In their study, they performed experiments of metastable wetting films on negatively charged, hydrophobic glass surfaces (gaseous phase methylated), or on hydrophilic, positively charged glass surfaces (with $\text{Al}^{3+}$ ions). Finally, Schulze (1984) reported the same range for aqueous 1,5-diaminohexane (DAH) films between an air bubble and a silica surface.

The phenomenon of thin film drainage and rupture has been studied in other different contexts. Chen (1984) analyzed the thin film that is trapped and forms a dimple between a horizontal solid surface and a small drop or bubble that approaches it, developing a model for an axisymmetric, dimple thinning film including the effects of London-van der Waals and
electric double layer forces. v. Klitzing (2005) reviewed the effect of the surface composition on forces within wetting films and aqueous foam. Coons et al. (2003) provided a thorough review of the drainage and spontaneous rupture in free standing thin films with tangentially immobile interfaces. Manev et al. (1997) proposed a new equation for the film thinning of microscopic foam films that fitted experimental data better. Barber and Hartland (1976) provided a rate of film thinning for the axisymmetric drainage of planar films. Jensen (1997) used the thin-film approximation, similarly to the procedure followed herein, to study the effects of surface tension on a thin layer lining in the interior of a cylindrical tube, where the tube has a centerline with weak, uniform curvature. This centerline curvature induces a pressure gradient in the thin film analogous to that due to a weak gravitational field. Hammond (1983) studied the stability of a thin annular film of viscous fluid surrounding a thread of another within a circular cylindrical pipe through a nonlinear analysis. Braun et al. (1999) used lubrication theory to derive an evolution equation for the free surface of a vertical draining free film due to gravitation. Howell et al. (2013) studied the flow of a thin liquid film along a flexible substrate where the gravity is the dominant driving force. The article is focused on steady solutions found with numerical and perturbation methods. Finally, Hahn and Slattery (1985) described the effects of surface viscosity on the stability of a draining plane parallel liquid film as a small bubble approaches a liquid-gas interface, until coalescence occurs. The authors used linear stability theory to study the phenomenon.

### 5.2.3 Current study

In this study, a drainage model and breakup criterion for the lubricating film of Taylor bubbles in slug flow in inclined round pipes is presented. Such criterion can be used to determine under which conditions the lubricating film is present, which is a key input for both numerical simulations (Hien and Fabre, 2004a; Taha and Cui, 2006; Ben-Mansour et al., 2010; Lizarraga-Garcia et al., 2015b) and mechanistic modeling of slug flow in order to determine correctly the Taylor bubble velocity and pressure drop. Also, it can be applied in flow assurance studies of high-viscosity oil slug flows, a critical aspect in oil and gas systems:
corrosion of the pipe material causes its blockage, and antioxidants are added to the liquid to avoid it. The prediction of a liquid film above the Taylor bubble so that antioxidants touch the entire pipe is thus key to guarantee their safety.

5.2.4 Film drainage

Figure 5-2 shows the geometry and frame of reference chosen for the analysis of the lubricating liquid film drainage. Let $u$, $v$, and $w$ denote the liquid film velocity in the azimuthal, radial, and longitudinal direction, respectively. Use of Cartesian coordinates is justified since $h/R \ll 1$. Thus, the Navier-Stokes equation in the $x$ direction is

$$
\frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} + \rho v \frac{\partial u}{\partial y} + \rho w \frac{\partial u}{\partial z} = -\frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + F_x(\phi),
$$

where $\mu$ is the liquid viscosity, $\rho$ is the liquid density, $p$ is the pressure, $F_x(\phi) = \rho g \cos(\theta) \sin(\phi)$ where $g$ is the gravity acceleration, and $\phi$ is the azimuthal angle with respect to the vertical. Equation 5.18 can be simplified using the lubrication approximation, by virtue of which
various terms can be neglected:

\[
\frac{\partial^2 u}{\partial x^2} \ll \frac{\partial^2 u}{\partial y^2}, \quad (5.19a)
\]

\[
\frac{\partial^2 u}{\partial z^2} \ll \frac{\partial^2 u}{\partial y^2}, \quad (5.19b)
\]

\[
\rho u \frac{\partial u}{\partial x} \ll \mu \frac{\partial^2 u}{\partial y^2}, \quad (5.19c)
\]

\[
\rho \frac{\partial u}{\partial t} \ll \mu \frac{\partial^2 u}{\partial y^2}, \quad (5.19d)
\]

Note that equation 5.19c applies equally to the other two inertia terms of the equation after
the continuity equation. Also, the pressure term can be neglected,

\[
\frac{\partial p}{\partial x} \approx 0, \quad (5.20)
\]

considering that the pressure differences inside the film due to gravity, surface tension and
DLVO forces are negligible, and the pressure inside the bubble is constant. The validity
of these approximations is verified later in section 5.2.4. Thus, the previous Navier-Stokes
equation 5.18 is simplified and, after imposing the no-slip at the wall and shear-stress-free
at the film surface boundary conditions, the azimuthal film velocity profile is found:

\[
u(\phi, y) = \frac{F_z(\phi)}{\mu} \left( hy - \frac{y^2}{2} \right), \quad (5.21)
\]

a parabolic profile whose approximate shape is depicted in figure 5-2c. Similarly, the Navier-
Stokes equation in the z direction is

\[
\rho \frac{\partial w}{\partial t} + \rho u \frac{\partial w}{\partial x} + \rho v \frac{\partial w}{\partial y} + \rho w \frac{\partial w}{\partial z} = -\frac{\partial p}{\partial z} + \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + F_z, \quad (5.22)
\]

where \( F_z = \rho g \sin(\theta) \). Note that \( v \) is much smaller than the other two velocity terms in this
lubrication approximation. Following an analogous procedure as in the x direction, equation

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5.22 is simplified and we obtain the longitudinal film velocity profile,

\[ w(\phi, y) = \frac{F_z}{\mu} \left( hy - \frac{y^2}{2} \right). \]  \hfill (5.23)

In order to obtain the governing PDE for the film drainage, the continuity equation is used:

\[ \frac{\partial h}{\partial t} + \frac{\partial Q'_x}{\partial x} + \frac{\partial Q'_z}{\partial z} = \frac{\partial h}{\partial t} + \frac{\partial}{\partial x} \int_0^h udy + \frac{\partial}{\partial z} \int_0^h wdy = 0, \]  \hfill (5.24)

where \( Q'_x \) and \( Q'_z \) are the volumetric flow per unit length in the \( x \) and \( z \) direction, respectively. Using equations 5.21 and 5.23, and recognizing that \( x = \phi \cdot R \), the second and third terms of the LHS of the previous equation can be developed:

\[
\begin{align*}
\frac{\partial Q'_x}{\partial x} &= \frac{\rho g \cos(\theta)}{\mu} h^2 \sin \left( \frac{x}{R} \right) \frac{\partial h}{\partial x} + \frac{\rho g \cos(\theta)}{3\mu R} h^3 \cos \left( \frac{x}{R} \right), \quad (5.25a) \\
\frac{\partial Q'_z}{\partial z} &= \frac{\rho g \sin(\theta)}{\mu} h^3 \frac{\partial h}{\partial z}. \quad (5.25b)
\end{align*}
\]

Noting that the three RHS terms of the previous equations are positive, and \( (\partial h/\partial z)/(\partial h/\partial x) \ll 1 \) by scaling analysis it can be concluded that

\[ \frac{\partial Q'_z}{\partial z} \ll \frac{\partial Q'_x}{\partial x}, \]  \hfill (5.26)

and therefore the film drainage PDE becomes

\[ \frac{\partial h}{\partial t} + \frac{\partial}{\partial \phi} \left( \frac{\rho g \cos(\theta) h^3}{3\mu R} \sin (\phi) \right) = 0. \]  \hfill (5.27)

The initial and boundary conditions are

\[
\begin{align*}
h(\phi, 0) &= h_i(\phi), \quad (5.28a) \\
\frac{\partial h(0, t)}{\partial \phi} &= 0. \quad (5.28b)
\end{align*}
\]
respectively, where equation 5.28b comes from the solution’s symmetry at $\phi = 0$. An analytical solution for equation 5.27 can be obtained at $\phi = 0$ using the method of characteristics through the Lagrange-Charpit equations (Delgado, 1997). After some simple algebra, the thin film drainage at $\phi = 0$ is

$$h(\phi = 0, t) = \left( \frac{1}{h_0^2} + \frac{2\rho g \cos(\theta)}{3\mu R} t \right)^{-1/2},$$

(5.29)

where $h_0 = h_i(\phi = 0)$. The evolution of the film thickness at $\phi = 0$, $h(\phi = 0, t)$, is key to determining when the film would break because that is the location of lowest thickness. To validate the analytical solution, equation 5.29 is compared with the numerical solution of equation 5.27 by a finite volume (FV) scheme implemented in MATLAB® (2013) using 4th-order Runge-Kutta for the time marching, and the Lax-Friedrichs flux, the latter defined as

$$f_{j+1/2} = \frac{1}{2} \left[ f(h_j) + f(h_{j+1}) - \alpha_{j+1/2}(h_{j+1} - h_j) \right] k(\phi_{j+1/2}),$$

(5.30)

where $f(h) = h^3$, $k(\phi) = \sin(\phi)$, and $\alpha_{j+1/2} = \max_{h_j,h_{j+1}} |f'(h)|$. Figure 5-3a shows they overlap perfectly for the high-viscosity oil whose properties are included in table 5.1. The nondimensional numbers used in table 5.1 are the Eötvös number $E_o = \rho g d^2 / \sigma$, the Morton number $M_o = g\mu^4 / (\rho \sigma^3)$, and the inverse viscosity number $N_f = \rho d^3 / 2 g^{1/2} / \mu$, where $d$ is the pipe diameter. Furthermore, it is important to note that $d\phi/dt \geq 0 \ \forall \ \phi \in [0, \pi]$ for the parameterized curve, which implies that the characteristics of the hyperbolic equation have positive slope and the information travels to the right along them, i.e., the right boundary does not affect the solution at $\phi = 0$. In particular, the solution for $h(\phi = 0, t)$ only depends on the initial condition at $\phi = 0$, $h_i(\phi = 0) = h_0$, and is independent from $h_i(\phi > 0)$. Figure 5-3b depicts the evolution of the numerical solution with time for the same high-viscosity oil for $\phi = [0, \pi/2]$ and three different initial film thicknesses, $h_{i,j}$, $j = 1, 2, 3$, where $h_{i,j}(\phi = 0) = h_0 \ \forall \ j$: a uniform film thickness, $h_{i,1} = h_0$; a linearly decreasing film thickness, $h_{i,2}(\phi) = h_0(1 - 0.9 \cdot \phi/(\pi/2))$; and a linearly increasing film thickness, $h_{i,3}(\phi) = h_0(1 + 0.9 \cdot \phi/(\pi/2))$. Three times are shown in the plot: $t = 0.01s$, 0.1s and 1s. The
Figure 5-3: (a) Comparison of the analytical and numerical solutions of equation 5.27 for a high-viscosity oil at $\phi = 0$, where time convergence is done with three time steps. Note that the analytical and numerical solutions overlap perfectly. (b) Numerical solution for $\phi = [0, \pi/2]$ for three different initial film thickness, $h_{i,j}$, $j = 1, 2, 3$, at $t = 0.01s$, 0.1s and 1s. The film thickness at $\phi = 0$, $h(\phi = 0, t)$, is independent from the initial film thickness at $\phi > 0$, $h_i(\phi > 0)$.

Table 5.1: Case study properties

<table>
<thead>
<tr>
<th>Case</th>
<th>$\rho$ [kg/m$^3$]</th>
<th>$\mu$ [Pa-s]</th>
<th>$\sigma$ [N/m]</th>
<th>$R$ [m]</th>
<th>$Eo$</th>
<th>$Mo$</th>
<th>$N_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kerosene</td>
<td>800</td>
<td>0.0016</td>
<td>0.028</td>
<td>0.025</td>
<td>700</td>
<td>3.7-10^{-9}</td>
<td>17,500</td>
</tr>
<tr>
<td>High-viscosity oil</td>
<td>885</td>
<td>0.4</td>
<td>0.03</td>
<td>0.0254</td>
<td>750</td>
<td>8.4</td>
<td>84</td>
</tr>
<tr>
<td>Water</td>
<td>999</td>
<td>0.001</td>
<td>0.072</td>
<td>0.0125</td>
<td>85</td>
<td>2.6-10^{-11}</td>
<td>12,000</td>
</tr>
</tbody>
</table>

film thickness at $\phi = 0$, $h(\phi = 0, t)$, coincides for the three cases at all times, which shows that equation 5.29 is valid independently of the initial film thickness at $\phi > 0$, $h_i(\phi > 0)$. It is also interesting to note that the initial conditions do not affect the solution at $t = 1s$ where the three solutions overlap.

Film drainage approximations validity

The validity of the lubrication approximation (equations 5.19) and negligible pressure change inside the film (equation 5.20) is proven here. Pipe geometries and fluids typical of slug flow such as high-viscosity oil, kerosene, and water (see table 5.1), are used to validate the
Table 5.2: Magnitude of the terms in equations 5.19 for the fluids of table 5.1, which justifies the lubrication approximation

<table>
<thead>
<tr>
<th>Case</th>
<th>Equation 5.19a</th>
<th>Equation 5.19b</th>
<th>Equation 5.19c</th>
<th>Equation 5.19d</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kerosene</td>
<td>2·10^{-5}</td>
<td>2·10^{-7}</td>
<td>5·10^{-3}</td>
<td>7·10^{-7}</td>
</tr>
<tr>
<td>High-viscosity oil</td>
<td>2·10^{-5}</td>
<td>2·10^{-7}</td>
<td>1·10^{-7}</td>
<td>1·10^{-11}</td>
</tr>
<tr>
<td>Water</td>
<td>6·10^{-5}</td>
<td>6·10^{-7}</td>
<td>4·10^{-2}</td>
<td>5·10^{-6}</td>
</tr>
</tbody>
</table>

In order to validate equation 5.20, the solution of the film thickness evolution accounting for the hydrostatic pressure and surface tension effects is successfully compared with the solution of equation 5.27. Also, the intermolecular forces are included through the intermolecular potential function in the liquid, $\Phi$, accounting for the difference behavior between a thin film and a bulk liquid (Reisfeld and Bankoff, 1992). To include these effects, we first look at the Navier-Stokes equation in the $y$ direction,

$$\rho \frac{\partial v}{\partial t} + \rho u \frac{\partial v}{\partial x} + \rho v \frac{\partial v}{\partial y} + \rho w \frac{\partial v}{\partial z} = -\frac{\partial (p + \Phi)}{\partial y} + \mu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + F_y(\phi) + \sigma \kappa \delta (y - h),$$

(5.31)

where $F_y(\phi) = \rho g \cos(\theta) \cos(\phi)$, $\delta$ is the Dirac delta function, and $\kappa = h''/(1 + h^2)^{3/2}$ is the curvature, where $h' = \partial h/\partial x$, and $h'' = \partial^2 h/\partial x^2$. Considering only van-der-Waals forces and neglecting electrical double layer interactions since there was no dilute electrolyte in the fluids studied, the intermolecular potential function, $\Phi$, is

$$\Phi = \frac{A}{6\pi h^3},$$

(5.32)

where $A$ is the Hamaker constant which is positive when attractive (Ruckenstein and Jain,
As a conservative estimate, \( A = 1 \cdot 10^{-19} \) J in this study (Israelachvili, 2011). Since \( v \) is much smaller than the other two velocity terms in this lubrication approximation, the equation can be simplified to

\[
0 = -\frac{\partial p}{\partial y} + F_y(\phi) + \sigma k \delta(y - h). \tag{5.33}
\]

Equation 5.33 can be integrated from \( y \) to \( h^+ \), where \( h^+ \) is located at the interface on the gas side:

\[
\int_y^{h^+} \frac{\partial p}{\partial y} dy = \int_y^{h^+} F_y(\phi) dy + \int_y^{h^+} \sigma k \delta(y - h) dy, \tag{5.34}
\]

that is

\[
p_{\text{gas}} - p = F_y(\phi)(h - y) + \sigma h'', \tag{5.35}
\]

where \( \kappa = h''/(1 + (h')^2)^{3/2} \approx h'' \). Equation 5.35 can be differentiated with respect to \( x \):

\[
\frac{\partial}{\partial x} (p_{\text{gas}} - p) = -\frac{\partial p}{\partial x} = F_y(\phi)\frac{h'}{R} - F_x(\phi)\frac{h - y}{R} + \sigma h''', \tag{5.36}
\]

where \( h'''' = \partial^3 h/\partial x^3 \). The Navier-Stokes equation in the \( x \) direction, equation 5.18, is slightly modified by adding the intermolecular potential term, \( \partial \Phi/\partial x = -Ah'/2\pi h^4 \). After some algebra, the azimuthal film velocity \( u \) becomes

\[
u(\phi, y) = \frac{F_x(\phi)(1 - h/R)}{\mu} + \frac{F_y(\phi)h' + \sigma h'''}{2\pi h^4} \left( hy - \frac{y^3}{2}\right) + \frac{F_x(\phi)}{2\mu R} \left( h^2 y - \frac{y^3}{3}\right), \tag{5.37}
\]

and the film drainage PDE is now

\[
\frac{\partial h}{\partial t} + \frac{\partial}{\partial \phi} \left( \left(F_x(\phi) (1 - h/R) + F_y(\phi)h' + \sigma h'' + \frac{Ah'}{2\pi h^4}\right) \frac{h^3}{3\mu R} + \frac{F_x(\phi)}{24\mu R^3} - \frac{5h^4}{24\mu R^2} \right) = 0. \tag{5.38}
\]

The initial and boundary conditions are the same as in equations 5.28. In order to solve equation 5.38, a finite difference (FD) scheme is implemented in MATLAB® (2013). MATLAB® ODE schemes for the time marching, and 2nd-order backward upwind schemes for the space derivatives are used. It is worth mentioning how the third derivative is calculated. For the
points on the right, $5 \leq i \leq N$ where $N$ is the number of points, a backward five stencil is used:

$$f'''(\phi_i) = \frac{3/2}{(\Delta \phi)^3} f(\phi_i - 4\Delta \phi) - \frac{7}{(\Delta \phi)^3} f(\phi_i - 3\Delta \phi) + \frac{12}{(\Delta \phi)^3} f(\phi_i - 2\Delta \phi) - \frac{9}{(\Delta \phi)^3} f(\phi_i - \Delta \phi) + \frac{5/2}{(\Delta \phi)^3} f(\phi_i).$$

(5.39)

$f'''(\phi)$ at the boundary points, $i = 1, 2$, are calculated through asymmetric backward five point stencil, that is, $f'''(\phi_1)$ at $\phi = 0$ is equal to

$$f'''(\phi_1) = -\frac{5/2}{(\Delta \phi)^3} f(\phi_1) + \frac{9}{(\Delta \phi)^3} f(\phi_2) - \frac{12}{(\Delta \phi)^3} f(\phi_3) + \frac{7}{(\Delta \phi)^3} f(\phi_4) - \frac{3/2}{(\Delta \phi)^3} f(\phi_5),$$

(5.40)

and $f'''(\phi_2)$ at $\phi = \Delta \phi$ is

$$f'''(\phi_2) = -\frac{3/2}{(\Delta \phi)^3} f(\phi_1) + \frac{5}{(\Delta \phi)^3} f(\phi_2) - \frac{6}{(\Delta \phi)^3} f(\phi_3) + \frac{3}{(\Delta \phi)^3} f(\phi_4) - \frac{1/2}{(\Delta \phi)^3} f(\phi_5).$$

(5.41)

For $i = 3$, $f'''(\phi_3)$ is calculated with a first order asymmetric backward four point stencil,

$$f'''(\phi_3) = -\frac{1}{(\Delta \phi)^3} f(\phi_1) + \frac{3}{(\Delta \phi)^3} f(\phi_2) - \frac{3}{(\Delta \phi)^3} f(\phi_3) + \frac{1}{(\Delta \phi)^3} f(\phi_4),$$

(5.42)

and $f'''(\phi)$ at $i = 4$ is calculated with a first order backward four point stencil,

$$f'''(\phi_4) = -\frac{1}{(\Delta \phi)^3} f(\phi_1) + \frac{3}{(\Delta \phi)^3} f(\phi_2) - \frac{3}{(\Delta \phi)^3} f(\phi_3) + \frac{1}{(\Delta \phi)^3} f(\phi_4),$$

(5.43)

Figure 5-4 shows the numerical solution of equation 5.38 (where $\partial \phi/\partial x \neq 0$) at $\phi = 0$ and the analytical solution (equation 5.29, $\partial \phi/\partial x = 0$) for high-viscosity oil and water, respectively. Also, figure 5-5 depicts the numerical solutions of equation 5.38 ($\partial \phi/\partial x \neq 0$) and equation 5.27 ($\partial \phi/\partial x = 0$) at four different times ($t = 1s, 10s, 150s, and 3,500s$ and $2,400s$) and $\phi = [0, \pi/2]$ for high-viscosity oil and water, respectively. Both numerical solutions are obtained with the same FD scheme. In all cases shown, the lines almost perfectly overlap, while the analytical solution sets a lower bound for the film thickness at initial times, and the van-der-Waals intermolecular force accelerates the drainage only when the film thickness
is on the order of 100nm. It is interesting to study which of the two terms in the RHS of equation 5.35 is dominant, which can be done through the film Eötvös number

\[
E_{\text{film}} = \frac{\Delta p_g}{\Delta p_\sigma} = \frac{\rho gh}{\sigma \kappa} = \frac{\rho gh}{\sigma h''/(1 + h'^2)^{3/2}}. \tag{5.44}
\]

For the three case studies of table 5.1, the \(E_{\text{film}}\) numerically calculated is such that \(E_{\text{film}} \gg 1\) for \(\phi \in [0, \pi/2]\) at every time, which means that the surface tension effects are negligible with respect to the hydrostatic term. As the film becomes thicker, the higher hydrostatic pressure opposes the liquid movement and reduces the film drainage, which explains why the film thickness values calculated with the analytical solution, equation 5.29, and the numerical solution of equation 5.27 are somewhat lower than those of the numerical solution of equation 5.38. This makes the criterion to avoid film breakup, equation 5.47, slightly more conservative, which is valid for its purpose. It is also worth mentioning that it is mainly the lower hydrostatic pressure closer to the wall that maintains the film attached to the pipe, and not the surface tension.
5.2.5 Film breakup criterion in Taylor bubbles of slug flow

As mentioned before, when the film drains to a critically low thickness, namely the critical thickness, $h_c$, it breaks. In this context, fluids typically present in oil and gas systems and nuclear reactors wet the pipe surfaces, thus, the capillary wave mechanism applies.

Based on this critical thickness, $h_c$, equation 5.29 can be non-dimensionalized:

$$\bar{h}(\phi = 0, \bar{t}) = \frac{h(\phi = 0, t)}{h_c} = \left( \left( \frac{h_c}{h_0} \right)^2 + \frac{t}{\tau} \right)^{-1/2} = \left( \left( \frac{h_c}{h_0} \right)^2 + \bar{t} \right)^{-1/2}, \quad (5.45)$$

where

$$\tau = \frac{3 \mu R}{2 \rho g \cos(\theta) h_c^2} \quad (5.46)$$

is the characteristic film drainage time. Figure 5-6 depicts the non-dimensional gravity-driven film thickness evolution for three different combinations of initial and critical film thicknesses, $h_0/h_c$. The three lines overlap after a certain time: an initial thicker film drains faster than a thinner one due to a higher gravitational force in comparison with the frictional one. Once they reach the same thickness, their drainage rate is the same. This can also be observed mathematically in equation 5.45, where $(h_c/h_0)^2$ becomes negligible with respect...
to the non-dimensional time, $\bar{t}$.

As explained above, film breakup occurs when the film drains to $h_c$, i.e., when $\bar{h} = 1$. For the applications described in section 5.2.3, it is important to establish a criterion for the film to remain above the bubble. To be certain that the film is not broken, we can impose that the film thickness should be ten times bigger than the critical thickness, $h/h_c = \bar{h} > 10$. Based on equation 5.45 and figure 5-6, and assuming that $h_0/h_c > 10$, this is satisfied when the time the film is draining is lower than $0.01\tau$. At a given pipe cross section, the film at $\phi = 0$ drains while the bubble is passing below (see figure 5-2b). Thus, the film drainage time is equal to the bubble’s passage time, $t_{\text{bubble}}$. Therefore, the criterion to avoid film breakup in Taylor bubble flow becomes:

$$\bar{t}_{\text{bubble}} < 0.01.$$  \hspace{1cm} (5.47)
5.2.6 Criterion application

In order to apply equation 5.47, the fluid properties, pipe geometry, and critical thickness are needed to calculate $\tau$ and the bubble's passage time. The critical film thickness can be estimated with equations 5.16 and 5.17, which characterize the capillary wave mechanism. Applying conservative estimates for the Hamaker constant, $h_c \sim 1 \mu m$ is a conservative critical film thickness value for the typical fluids shown in table 5.1, high-viscosity oil, kerosene, and water, and steel pipe. The correlation of Llewelin et al. (2012) for vertical pipes in stagnant liquid gives a film thickness, $h$, equal to 13, 2.4 and 0.67 mm, respectively. These numbers can be used to estimate the order of magnitude of the initial film thicknesses as $h_0 = h/10$, which are much larger than the estimated critical thickness. Finally, the Taylor bubble passage time can be estimated as the inverse of the slug frequency given by models of slug flow (Gregory and Scott, 1969; Zabaras, 2000; Gokcal et al., 2009a; Hernandez-Perez et al., 2010), or by employing Taylor bubble velocity models (Viana et al., 2003; Hayashi et al., 2010, 2011; Kurimoto et al., 2013; Lizarraga-Garcia et al., 2015a) and an estimated length for individual bubbles. The latter is applied in Section 4.2 of Chapter 6.

5.2.7 Experimental validation

In order to validate the film drainage and breakup model, experiments of Taylor bubbles in inclined pipes with stagnant liquid are performed. There, the drainage time until the lubricating film breaks, $t_{\text{breakup}}$, is measured for different liquids and inclination angles (see figure 5-7). This breakup occurs when $\tilde{h} = 1$. Based on equation 5.45, and assuming that $h_0/h_c \gg 1$, this corresponds to a non-dimensional drainage time, $\tilde{t}_{\text{breakup}}$, equal to 1, that is,

$$\tilde{t}_{\text{breakup}} = \frac{t_{\text{breakup}}}{\tau} = \frac{t_{\text{breakup}}}{\frac{3\mu R}{2\rho g \cos \theta h_c^2}} = 1.$$  (5.48)
Figure 5-7: Example of the film breakup for a 50% DI water-50% methanol mixture at \( \theta = 15^\circ \) inclination. The shaded line indicates the film rupture front.

All the values of this equation but the breakup film thickness, \( h_c \), are experimentally measured. Based on equation 5.48, the reported quantity

\[
\frac{t_{\text{breakup}}}{h_c^2} = \frac{t_{\text{breakup}}}{\frac{3\mu R}{2pg\cos(\theta)}h_c^2} = \frac{t_{\text{breakup}}}{\frac{3\mu R}{2p_g\cos(\theta)}} = \frac{1}{h_c^2}
\] (5.49)

should be constant for every inclination angle and each liquid. Thus, an estimate of the film critical thickness can be obtained from the experimental measurements,

\[
h_c = \sqrt{\frac{3\mu R}{2pg\cos(\theta)}} t_{\text{breakup}}
\] (5.50)

The experimental setup, shown in figure 5-8, consists of a High Speed Camera (HSC), a compressor, a polycarbonate tube of diameter \( d = 0.0127 \text{ m} \), and three valves. The inclination angles studied are \( \theta = 5^\circ, 15^\circ, 30^\circ, 37.5^\circ, 45^\circ, 60^\circ, 75^\circ, \) and \( 90^\circ \). The liquids used are methanol, ethanol, and three mixtures of DI water and methanol, whose properties are measured at the beginning and end of each experiment. These properties and the experimental techniques used are shown in table 6.1, where the mixture percentages are volumetric.
The experimental procedure is as following: first, air at atmospheric pressure is introduced and held between the closed valves at "b" and "c". Then, valve "c" is opened and the Taylor bubble advances up through the tube due to buoyancy. The HSC records the bubble movement once it has reached its terminal velocity and generates the images shown in figure 5-7. The experiment finishes when the bubble reaches point "d". To rerun the experiment, the liquid contained between valves "b" and "c" is replaced by air at atmospheric pressure: the compressor pushes the liquid from "a" to "d" through the capillary tube while valve "c" is closed, and valve "b" open. Since "d" is connected to atmosphere, compartment "b"-"c" remains at atmospheric pressure once the compressor is turned off. The closing of valve "b" confines the air at atmospheric pressure in this compartment so that the experiment can be performed again.

Five experiments are performed for each liquid and inclination angle. For certain liquids and inclination angles, film breakup does not occur and thus \( t_{breakup} \) cannot be measured. In the present experimental setup, the film of ethanol and methanol does not break up at any inclination angle: both liquids wet polycarbonate effectively, as their contact angle values indicates in table 6.1, making the critical film thickness, \( h_c \), low enough so that it is not
reached during the gravity-driven drainage.

On the other hand, film breakup occurs for the mixtures of DI water and methanol. The HSC pictures of figure 5-7 show that the visually observable film breakup occurs at the top of the tube, $\phi = 0$, where the film is the thinnest, consistent with the present model. Table 5.4 reports the measured $\bar{t}_{\text{breakup}}/h_c^2$ values, the calculated $h_c$ values (equation 5.50), and the maximum inclination angle at which breakup occurs, $\theta_{\text{breakup, max}}$, for each liquid. For the 50% DI water-50% methanol mixture, film breakup occurs up to 60° inclination angle. For higher angles, the film does not drain enough to reach $h_c$ and break. The values of $\bar{t}_{\text{breakup}}/h_c^2$ are scattered along an approximately constant value, as shown in figure 5-9. The experimental error, less than 10% the value of $\bar{t}_{\text{breakup}}/h_c^2$, is much smaller than the repeatability error, thus only the latter is reported. For the 37.5% DI water-62.5% methanol mixture, film breakup occurs only at 5 and 15° inclination angles, and the values of $\bar{t}_{\text{breakup}}/h_c^2$ are higher than those of the previous mixture, that is, the critical film thickness $h_c$ is higher for the latter mixture, as inferred by its lower contact angle. Finally, the 25% DI water-75% methanol mixture only experiences film breakup at 5° inclination angle, and the value of $\bar{t}_{\text{breakup}}/h_c^2$ is again higher than the previous two mixtures, in accordance with its lower contact angle measured. The calculated critical thicknesses, $h_c$, are 24μm for the 25% DI water-75% methanol mixture, 35μm for the 37.5% DI water-62.5% methanol mixture, and 44μm for the 50% DI water-50% methanol mixture. The order of magnitude of these values coincides with the film thickness magnitude reported by Behafarid et al. (2015); Podowski and Hirsa (2001) and Podowski and Kumbaro (2004), 50 to 100 μm, who studied theoretically and experimentally this phenomenon. Note that these values are slightly higher than the critical thickness estimation done in Section 5.2.6. The discrepancy is due to differences in the contact angle, which affects the film breakup mechanism and magnitude (Stöckelhuber, 2003; Stöckelhuber et al., 2004). The contact angle between the typical fluids of the systems mentioned (oil and gas, nuclear) and steel pipes, below 10° (Coriand et al., 2015; Kamura et al., 2009), is much lower than in the experiments where the film breaks up, 40-55°. The experimental results have also been statistically analyzed: the Kolmogorov-Smirnov and Shapiro-Wilk tests state
Table 5.3: Experimental liquid properties

<table>
<thead>
<tr>
<th>Liquid</th>
<th>( \rho ) [kg/m(^3)]</th>
<th>( \mu ) [Pa-s]</th>
<th>( \sigma ) [N/m]</th>
<th>Contact angle [°]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol</td>
<td>789</td>
<td>0.0011</td>
<td>0.022</td>
<td>0-5</td>
</tr>
<tr>
<td>Methanol</td>
<td>791.8</td>
<td>0.00058</td>
<td>0.022</td>
<td>1-5</td>
</tr>
<tr>
<td>25% DI water-75% Methanol</td>
<td>865.8</td>
<td>0.0014</td>
<td>0.024</td>
<td>40</td>
</tr>
<tr>
<td>37.5% DI water-62.5% Methanol</td>
<td>882.8</td>
<td>0.0015</td>
<td>0.025</td>
<td>45</td>
</tr>
<tr>
<td>50% DI water-50% Methanol</td>
<td>921.2</td>
<td>0.0018</td>
<td>0.031</td>
<td>55</td>
</tr>
<tr>
<td>Measurement technique</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Calibrated volume weight</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Capillary viscometer</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pending drop</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sessile drop</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 5.4: Experimental results, where values in parenthesis indicate standard deviation. Note that while \( h_c \) does not depend on \( \theta \), film breakup is not observed for \( \theta > \theta_{\text{breakup, max}} \) as the film does not drain enough to reach that value.

<table>
<thead>
<tr>
<th>Liquid</th>
<th>( \bar{t}_{\text{breakup}}/h_c^2 ) [1/m(^2)]</th>
<th>( h_c ) [μm]</th>
<th>( \theta_{\text{breakup, max}} ) [°]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Methanol</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>25% DI water-75% Methanol</td>
<td>1.7\times10^9 (4\times10^8)</td>
<td>24 (3)</td>
<td>5</td>
</tr>
<tr>
<td>37.5% DI water-62.5% Methanol</td>
<td>8.3\times10^8 (2.1\times10^8)</td>
<td>35 (5)</td>
<td>15</td>
</tr>
<tr>
<td>50% DI water-50% Methanol</td>
<td>5.2\times10^8 (2.2\times10^8)</td>
<td>44 (9)</td>
<td>60</td>
</tr>
</tbody>
</table>

that the data \( \bar{t}_{\text{breakup}}/h_c^2 \) of each liquid follow a normal distribution around the mean shown in table 5.4.

### 5.2.8 Conclusions

In summary, it is important to predict under which conditions the lubricating film above a Taylor bubble in slug flow is present. In this section, an analytical model predicting the gravity-induced drainage of the thin film is presented, and from it a criterion to avoid the film breakup is derived: \( \bar{t}_{\text{bubble}} = t_{\text{bubble}}/\tau < 0.01 \). The model has been experimentally validated through Taylor bubbles in inclined pipes with stagnant liquids. The application of this criterion to the present simulations is done in section 6.3.2, chapter 6.
Figure 5-9: $\bar{t}_{\text{breakup}}/h_c^2$ values are scattered along an approximately constant value, from which the critical film thickness is calculated, $h_c = 44\mu m$.

5.3 Effect of Taylor bubble length on its terminal velocity and shape in inclined pipes

It is well known that the dynamics of Taylor bubbles in vertical pipes are independent of their length (Griffith and Wallis, 1961; Llewellin et al., 2012; Mao and Dukler, 1989; Tomiyama et al., 2001). However, the effect of bubble length in inclined pipes has only been mentioned by Zukoski (1966), who stated that, in his experiments, “the propagation velocity is independent of length as long as the volume of the bubble corresponds to a cylinder with the tube radius and a length of three tube radii”. Here, we present both experiments and simulations showing that not only the terminal velocity but also the Taylor bubble shape are independent of its length in inclined pipes.

5.3.1 Experiments

We measure the terminal velocity of Taylor bubbles with different volumes in inclined pipes. We analyze four liquids (methanol, ethanol, DI water, and a mixture of 50% DI water
and 50% methanol in volume) at five inclination angles (θ = 5°, 15°, 30°, 37.5°, 45°). The experimental setup used is the one shown before in figure 5-8. For each liquid and inclination angle, several measurements are taken. In the first five measurements, \( i = 1, \ldots, 5 \), valve “c” is maintained open and the compartment “b”-“c” fills up completely with liquid. In the following measurements, \( i > 5 \), valve “c” is closed progressively earlier in time so that air remains in the compartment “b”-“c” and the volume of the experimental bubble rising the tube is progressively smaller, \( V_i > V_{i+1} \). The bubble images obtained with the HSC are post-processed in MATLAB® to calculate the terminal velocity based on the position of the bubble tip. Figure 5-10 shows an example for the mixture of 50% DI water and 50% methanol, and \( \theta = 15° \), where the upper figure is the bubble picture taken with the HSC, the middle figure is the post-processed image, and the lower plot depicts the bubble tip position versus time and the linear fitted line. For every experiment, the linear fit between the bubble tip position and time provides a 2\( \sigma \) value of less than 0.1% the terminal velocity, \( v_t \), and a coefficient of determination \( R^2 = 1 \), which means that steady state is reached. For all four fluids and five inclination angles, the measured terminal velocity was found to vary by no more than 1% when the bubble volume was varied up to 85% with respect to \( V_1 \), corresponding to approximately the same bubble length variation. For each liquid and inclination angle, the Kolmogorov-Smirnov statistical test states that the measured data, \( v_i \), comes from the same normal distribution \( N(\bar{v}, s) \), where the mean is calculated as \( \bar{v} = \sum_{i=1}^{n} v_i / n \), and the standard deviation as \( s = (\sum_{i=1}^{n} |v_i - \bar{v}|^2 / (n - 1))^{1/2} \), where \( n \) is the number of measurements for that configuration. Figure 5-11 shows the residuals, \( |v_i - \bar{v}| / \bar{v} \), for methanol (a), the mixture of 50% DI water and 50% methanol (b), ethanol (c), and DI water (d). It can be observed that bubble volume does not affect the residuals. This indicates that the bubble volume and length do not affect significantly the terminal velocity.

We also used the experiments to verify the accuracy of the bubble shape predicted by the simulations. The bubble tip of two different volumes is compared with the one obtained in simulations for the mixture of 50% DI water and 50% methanol. Figures 4-12 to 4-16 of
Figure 5-10: Experimental bubble image post-processing to obtain the bubble terminal velocity, \( v_t \), for the mixture of 50% DI water and 50% methanol, \( \theta = 15^\circ \), and measurement 1, i.e., \( i = 1 \).

section 4.3.2, chapter 4, depict the shape comparison for \( \theta = 45^\circ, 37.5^\circ, 30^\circ, 15^\circ \), and \( 5^\circ \), respectively. Bubble volume \( V_1 \) is characterized by \( \lambda = 3.5 \), where parameter \( \lambda \) is calculated as \( \lambda = d_e / d \), where \( d_e \) is the sphere-volume equivalent diameter of the bubble. Bubble volume \( V_2 \) is characterized by \( \lambda = 2.3 \) for \( \theta = 45^\circ \), \( \lambda = 2.2 \) for \( \theta = 37.5^\circ, 5^\circ \), and \( \lambda = 2.4 \) for \( \theta = 30^\circ, 15^\circ \). Finally, the simulated bubble volumes are characterized by \( \lambda = 1.4 \) for \( \theta = 45^\circ, 37.5^\circ \), \( \lambda = 1.3 \) for \( \theta = 30^\circ, 15^\circ \), and \( \lambda = 1.2 \) for \( \theta = 5^\circ \). It can be seen that the bubble tip shapes overlap very well.

### 5.3.2 Simulations

Numerical simulations also confirm that the terminal velocity and bubble shape do not depend on the bubble volume/length. Here we analyze a fluid with \( Mo = 19 \) and \( Eo = 31 \) at two inclination angles (\( \theta = 60^\circ, 45^\circ \)). Bubble volumes are characterized by \( \lambda = 1.05, 1.17 \).
The differences between the terminal velocities of both volumes are 0.07% and 0.2% for $\theta = 60^\circ$ and $\theta = 45^\circ$, respectively. Furthermore, Figure 5-12 shows that the bubble tip shapes overlap for both inclination angles.

### 5.3.3 Conclusions

Based on these results, it is concluded that the Taylor bubble length does not affect its dynamics in inclined pipes, which is an important assumption made in the simulations described in chapters 6 and 7.
Figure 5-12: Taylor bubble shapes in a liquid with $Mo = 19$ and $Eo = 31$ overlap for two different bubble volumes ($\lambda = 1.17, 1.05$) for $\theta = 60^\circ$ (a) and $\theta = 45^\circ$ (b)

5.4 Conclusions

In this chapter, the two main assumptions used in the simulations of the study were presented: the lubricating liquid film formed above the bubble as the pipe inclines with respect to the horizontal does not breakup, i.e., the gas phase never touches the pipe and triple line is not formed; and the Taylor bubble length does not affect its dynamics in inclined pipes. To verify the robustness of the first assumption, the gravity-induced film drainage was analytically modeled and experimentally validated. From it a criterion to avoid film breakup was obtained, which holds in the simulations performed. The second assumption was validated with both experiments and simulations.
Chapter 6

Taylor Bubbles in Inclined Pipes with Stagnant Liquid

6.1 Introduction

Two-phase slug flow is a common occurrence in wells, riser pipes and pipelines of crude oil and natural gas systems. Current predictive tools for two-phase flow are based on either the mixture model or the mechanistic two-fluid model Brill and Mukherjee (1999). In the latter, slug flow is modeled as a sequence of fundamental units, also called slug units. Each unit contains a long bullet-shaped bubble, known as Taylor bubble, and a liquid portion with smaller homogeneously distributed bubbles, known as liquid slug. Thorough studies about the modeling of two-phase slug flow can be found in Bendiksen et al. (1996); Fabre and Liné (1992); Taitel and Barnea (1990). The mechanistic model requires the use of closure relations to capture the transfer of mass, momentum and energy between the phases, in the respective conservation equations, so that integral flow parameters such as liquid holdup (or void fraction) and pressure gradient can be predicted. However, these closure relations typically carry the highest uncertainties in the model, since they are obtained empirically or
through the use of overly simplified assumptions. In particular, significant discrepancies have
been found between experimental data and closure relations for the Taylor bubble velocity
in slug flow, which has been determined to strongly affect the pressure gradient and liquid
holdup predicted by the mechanistic models of Ansari et al. (1994); Orell and Rembrand
(1986); Petalas and Aziz (2000).

Taylor bubble velocity, $v_{TB}$, in slug flow is generally modeled based on the drift flux
approach of Nicklin et al. (1962),

$$v_{TB} = C_0 \cdot v_m + v_d,$$  \hspace{1cm} (6.1)

where $v_d$ is the drift velocity of the bubble in a stagnant liquid, and $C_0 \cdot v_m$ is the contribution
of the mixture velocity, $v_m$, which is the sum of the liquid and gas superficial velocities,
$v_m = v_{SL} + v_{Sg}$. The distribution parameter, $C_0$, is a dimensionless coefficient that captures
the effect of nonuniform flow and void concentration profiles. The latter is analyzed in detail
in the following chapter, while the present chapter is focused on the velocity and dynamics
of the Taylor bubble in stagnant liquid, i.e., the second term of the RHS of equation 6.1, $v_d$.

Taylor bubble’s dynamics are influenced by the viscous, inertial, gravitational, and inter-
facial forces acting on it. Assuming that the liquid transport properties are dominant
($\rho_g/\rho_L \ll 1$, $\mu_g/\mu_L \ll 1$, where the subscripts $g$ and $L$ indicate the gas and liquid phases,
respectively, $\rho$ is the density, and $\mu$ is the dynamic viscosity), dimensional analysis indicates
the following four dimensionless $\pi$-groups are sufficient to determine the bubble dynamics:
the Froude number, $Fr = \frac{v_{TB}}{\sqrt{gd}}$, where $g$ is the gravitational acceleration and $d$ is the
pipe diameter, is the ratio of the bubble inertia to the gravitational forces; the Eötvös num-
ber, $Eo = \frac{\rho L g d^2}{\sigma}$, $\sigma$ is the surface tension, is the ratio of the gravitational to interfacial
forces; the Morton number, $Mo = \frac{g \mu_L^4}{\rho_L \sigma^3}$, sometimes called the property number; and
the inclination angle, $\theta$, measured from the horizontal. Note, however, that the choice of
the $\pi$-groups is not unique; for example, the inverse viscosity number, $N_f$, a combination
of $Eo$ and $Mo$, can also be employed. Thus, Buckingham $\Pi$-Theorem assures that the four
$\pi$-groups are related by a unique function of the form $Fr = f(Eo, Mo, \theta)$. In this chapter,
a proposed correlation for this function is presented for an ample range of fluid properties and pipe inclination angles: $Eo \in [10, 700]$, $Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^3]$, and $\theta \in [0^\circ, 90^\circ]$.

6.2 Literature review

The literature for Taylor bubbles rising in vertical tubes ($\theta = 90^\circ$) filled with a stagnant liquid is extensive. Davies and Taylor (1950) and Dumitrescu (1943) studied analytically the limiting problem of negligible viscous force and surface tension where $Fr$ is found to be constant. White and Beardmore (1962) performed a wide range of experiments and proposed a general graphical correlation of $Fr$ as a function of $Eo$ and $Mo$, identifying regions where some governing forces can be neglected (see figure 6-1). Zukoski (1966) investigated experimentally the influence of liquid viscosity and surface tension on the bubble velocity, and proposed a velocity correlation for vertical tubes. Wallis (1969) reported a correlation with three different regions based on $Nf$ for the vertical drift velocity, $v^v_d$, and a horizontal drift velocity, $v^h_d$:

$$v^h_d = \left(0.54 - \frac{1.76}{Eo^{0.56}}\right) \sqrt{\frac{gd(\rho_L - \rho_g)}{\rho_L}}, \quad (6.2a)$$

$$v^v_d = 0.345 \left(1 - e^{-0.01Nf/0.345}\right) \left(1 - e^{(3.37 - Eo)/m}\right) \sqrt{\frac{gd(\rho_L - \rho_g)}{\rho_L}}, \quad (6.2b)$$

$$m = \begin{cases} 
10, & \text{if } Nf > 350, \\
69N_f^{-0.35}, & \text{if } 350 > Nf > 18, \\
25, & \text{if } 18 > Nf. 
\end{cases} \quad (6.2c)$$

Viana et al. (2003) performed experiments and, together with the available published data, obtained a correlation for $Fr = f(Nf, Eo)$. They composed bi-power laws for two separate flow regions: large $Nf$, $Nf > 200$, and small $Nf$, $Nf < 10$, and connected them through a
logistic dose response curve (Patankar et al., 2002; Joseph and Yang, 2010):

\[
Fr = \frac{0.34}{(1 + (14.793/Eo)^{3.06})^{0.58}} \left(1 + \left(\frac{N_f}{31.08(1 + (29.868/Eo)^{1.96})^{0.49}}\right)^a\right)^b 
\]

\[
a = -1.45(1 + (24.867/Eo)^{9.93})^{0.94}
\]

\[
b = -1.0295/a.
\]

CFD numerical simulations have also been used to study slug flow mainly with 2D axisymmetric domain. Clarke and Issa (1997), and Mao and Dukler (1990) focused on the flow ahead and around the bubble. Araújo et al. (2012) analyzed a wide range of Taylor bubbles in vertical stagnant liquid columns using 2D axisymmetric simulations \((Eo \in [6, 900], Mo \in [4.72 \times 10^{-5}, 104], N_f \in [3.5, 517])\). Araújo et al. (2013) studied the hydrodynamics of pairs of consecutive Taylor bubbles in stagnant liquid. Kurimoto et al. (2013) studied experimentally and numerically the terminal velocities of clean and contaminated drops, as well as Taylor bubbles, in vertical pipes. In their terminal velocity correlation, they modified the coefficients of the correlations given by Hayashi et al. (2011), who obtained the functional form of that empirical correlation through a force balance on the Taylor drop. The latter was deduced with a scaling analysis based on the field equations for two phases and the jump conditions at the interface. The range of applicability of their correlation is \(Eo \in [4.8, 228]\) and \(Mo \in [1 \times 10^{-12}, 1 \times 10^4]\). Taha and Cui (2006) performed both 2D axisymmetric and 3D simulations of vertical pipes with stagnant fluid, reporting that the bubble wake becomes non-axisymmetric for \(N_f > 500\). Ramdin and Henkes (2012) performed simulations using VOF, including some limiting cases for inviscid liquid \((Mo = 0, N_f = \infty)\), and zero surface tension \((Eo = \infty)\). Other 2D vertical axisymmetric studies were done by Bugg et al. (1998) and Kang et al. (2010).

The effect of the pipe inclination angle on the Taylor bubble dynamics has also been studied in the literature. Table 6.1 shows the \(Eo\) and \(Mo\) number ranges of these studies as well as the inclination angles covered, and Figure 6-1 locates these experimental data in the map of White and Beardmore (1962). Zukoski (1966) described qualitatively the effect
of tube inclination in closed tubes. Bendiksen (1984) was the first to propose a correlation for inclined pipes:

\[ v_d = v_d^h \cos \theta + v_d^v \sin \theta, \quad (6.4a) \]
\[ v_d^v = 0.351 \sqrt{gd}, \quad (6.4b) \]
\[ v_d^h = 0.542 \sqrt{gd}. \quad (6.4c) \]

He claimed that \( v_d^h \) can be different from zero in pipes with one end opened and partially filled with liquid and gas. In the open end, liquid drains out and gas enters the pipe, which moves the bubble forward inside due to the differences in liquid level at both sides of the bubble. These assumptions conflict with previous investigations of Nicklin et al. (1962) and Dukler and Hubbard (1975), who assumed \( v_d^h = 0 \) in a closed horizontal pipe. Weber et al. (1986) developed an ample experimental study covering \( Eo \in [4.9 - 490] \) and \( Mo \in [2.2 \cdot 10^{-11}, 1.5 \cdot 10^4] \). Furthermore, they proposed a correlation with a correction term \( Q \) which is a function of \( \Delta Fr_d = Fr_d^v - Fr_d^h \):

\[ Fr_d = Fr_d^h \cos \theta + Fr_d^v \sin \theta + Q, \quad (6.5a) \]
\[ Q = \begin{cases} 
1.37 (\Delta Fr_d)^{2/3} \sin \theta (1 - \sin \theta), & \text{if } \Delta Fr_d > 0, \\
0, & \text{if } \Delta Fr_d \leq 0. 
\end{cases} \quad (6.5b) \]

In their article, \( Fr_d^v \) and \( Fr_d^h \) are obtained by interpolation of the experimental data, and they give a graphical general dimensionless correlation for horizontal tubes. Hasan and Kabir (1988a) performed an experimental study for \( \theta \in [58^o, 90^o] \) and proposed a new correlation for bubble velocity in stagnant liquid:

\[ v_d = v_d^v \sqrt{\sin \theta (1 + \cos \theta)^{1.2}}, \quad (6.6a) \]
\[ v_d^v = 0.35 \sqrt{gd}, \quad (6.6b) \]

where equation 6.6b is there justified for systems with large \( N_f \) and \( Eo \) values (e.g., \( N_f > 300 \)).
and $Eo > 100$) where $Fr_d$ becomes constant. Furthermore, they assumed $v_d^h = 0$. Spedding and Nguyen (1978) and Alves et al. (1993) studied experimentally and analytically, the surface tension effects on the velocity of Taylor bubbles in inclined pipes, for which they used water and kerosene. Carew et al. (1995) derived a semi-theoretical expression for the rise velocity of air bubbles in inclined pipes of stagnant water, and performed experiments with non-Newtonian fluids. Petalas and Aziz (2000) used the correlations of Wallis (1969) for the horizontal drift velocity (equation 6.2a), and a modification of their vertical drift velocity, equation 6.2b:

$$v_d^h = \left(0.54 - \frac{1.76}{Eo^{0.36}}\right) \sqrt{\frac{gd (\rho_L - \rho_g)}{\rho_L}},$$  \hfill (6.7a)

$$v_d^v = 0.345 \left(1 - e^{-Eo \exp(3.278 - 1.424 \ln Eo)}\right) \sqrt{\frac{gd (\rho_L - \rho_g)}{\rho_L}},$$  \hfill (6.7b)

$$v_d = f_m \left(v_d^h \cos \theta + v_d^v \sin \theta\right),$$  \hfill (6.7c)

where $f_m = \min \left(0.316\sqrt{\frac{d \rho_d \nu_{\infty}}{2 \mu_L}}, 1\right)$ is obtained from Zukoski (1966). Shoso and Ryan (2001) studied experimentally the motion of long bubbles in inclined tubes for $5^\circ$ to $90^\circ$ inclination angles, for Newtonian and non-Newtonian fluids. Gokcal et al. (2009b) investigated experimentally the effect of high oil viscosity on drift velocity for horizontal and inclined pipes using water and viscous oil. They proposed a new correlation for the horizontal drift velocity extending the analysis of Benjamin (1968) to include viscosity, and used the expression of Joseph (2003) for the vertical drift velocity:
\begin{align*}
\frac{h}{d} &= 0.1038 \ln \mu_L + 0.9684, \quad (6.8a) \\
\frac{S}{d} &= \sqrt{1 - (2h/d - 1)^2}, \quad (6.8b) \\
\gamma_1 &= \begin{cases} 
\frac{\pi}{2} - \sin^{-1}\left(\frac{S}{d}\right), & \text{if } h/d < 0.5, \\
\sin^{-1}\left(\frac{S}{d}\right), & \text{if } h/d \geq 0.5,
\end{cases} \quad (6.8c) \\
\gamma &= \min(\gamma_1, 1.444784), \quad (6.8d) \\
\zeta &= \frac{(\gamma - 0.5 \sin 2\gamma)}{\pi}, \quad (6.8e) \\
\Delta &= \frac{1 + \zeta}{\zeta} \left(\frac{d}{2}(1 - \cos \gamma) - \left(\frac{3}{2} \left(1 - (1 - \zeta) \cos \gamma - 2(\sin \gamma)^3 / 3\pi\right)\right)^{1/2} - 2\right), \quad (6.8f) \\
v_2 &= \sqrt{2g \left(\frac{d}{2}(1 - \cos \gamma) - \Delta\right)}, \quad (6.8g) \\
v_d^h &= (1 - \zeta)v_2, \quad (6.8h) \\
v_d^v &= -\frac{8}{3} \frac{\mu_L}{\rho_L d} + \sqrt{\frac{2}{9} g d + \frac{64}{9} \left(\frac{\mu_L}{\rho_L d}\right)^2}, \quad (6.8i) \\
v_d &= v_d^h(\cos \theta)^{1.5} + v_d^v(\sin \theta)^{0.7}. \quad (6.8j)
\end{align*}

Jeyachandra et al. (2012) analyzed experimentally the Taylor bubble terminal velocity for high-viscosity oil, proposing a new horizontal drift velocity. They also used the expression of Joseph (2003) for the vertical drift velocity:

\begin{align*}
Fr_d &= Fr_d^h \cos \theta + Fr_d^v \sin \theta, \quad (6.9a) \\
Fr_d^v &= \frac{8}{3} N_f^{-1} + \sqrt{\frac{2}{9} \frac{\rho_L}{\rho_L - \rho_g} + \frac{64}{9} N_f^{-2}}, \quad (6.9b) \\
Fr_d^h &= 0.53 \exp \left(-13.7 N_f^{-0.46} E_0^{-0.1}\right). \quad (6.9c)
\end{align*}

Moreiras et al. (2014) conducted experiments with medium viscosity oils \((Eo = 804, Mo \in \left[1.25 \cdot 10^{-3}, 0.41\right])\) for inclination angles between \(0^\circ\) and \(90^\circ\). Moreover, they proposed a unified dimensionless closure relationship for drift velocity using data from the literature as well as theirs. Similar to the correlation of Weber et al. (1986) (equations 6.5), they used a
Table 6.1: Experimental studies of Taylor bubbles in inclined pipes with a stagnant fluid

<table>
<thead>
<tr>
<th></th>
<th>$\theta$ [°]</th>
<th>$E_0$</th>
<th>$M_o$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zukoski (1966)</td>
<td>0 – 90</td>
<td>3.48 – 4,000</td>
<td>2.59·10⁻¹¹ – 19.2</td>
</tr>
<tr>
<td>Spedding and Nguyen (1978)</td>
<td>0 – 90</td>
<td>50 – 10,000</td>
<td>~2.59·10⁻¹¹</td>
</tr>
<tr>
<td>Bendiksen (1984)</td>
<td>0 – 90</td>
<td>50 – 340</td>
<td>~2.63·10⁻¹¹</td>
</tr>
<tr>
<td>Weber et al. (1986)</td>
<td>0 – 90</td>
<td>4.9 – 490</td>
<td>2.2·10⁻¹¹ – 1.5·10⁴</td>
</tr>
<tr>
<td>Hasan and Kabir (1988a)</td>
<td>58 – 90</td>
<td>2,200</td>
<td>~2.63·10⁻¹¹</td>
</tr>
<tr>
<td>Alves et al. (1993)</td>
<td>0 – 90</td>
<td>800</td>
<td>3.66·10⁻⁶</td>
</tr>
<tr>
<td>Shosho and Ryan (2001)</td>
<td>5 – 90</td>
<td>21.9 – 629</td>
<td>2.17·10⁻¹¹ – 6.11·10⁴</td>
</tr>
<tr>
<td>Gokcal et al. (2009b)</td>
<td>5 – 90</td>
<td>349; 776</td>
<td>2.63·10⁻¹¹; 5.30·10⁻¹ – 1.24·10³</td>
</tr>
<tr>
<td>Jeyachandra et al. (2012)</td>
<td>0 – 90</td>
<td>765 – 6,970</td>
<td>0.258 – 49.2</td>
</tr>
<tr>
<td>Moreiras et al. (2014)</td>
<td>0 – 90</td>
<td>804</td>
<td>1.25·10⁻³ – 0.41</td>
</tr>
<tr>
<td>Present study</td>
<td>0 – 90</td>
<td>10 – 700</td>
<td>1 · 10⁻⁶ – 5 · 10³</td>
</tr>
</tbody>
</table>

correction factor $Q$ dependent on $\Delta Fr_d = Fr_d^v - Fr_d^h$. Furthermore, they introduced four parameters, $a = 1.2391$, $b = 1.2315$, $c = 2.1589$, $d = 0.70412$, in order to fit the data:

$$Fr_d = Fr_d^h \cos^a \theta + Fr_d^v \sin^b \theta + Q,$$

(6.10a)

$$Fr_d^v = -\frac{8}{3} N_f^{-1} + \frac{2}{9} \frac{\rho_L}{\rho_L - \rho_g} + \frac{64}{9} N_f^{-2} \left( \frac{\sqrt{2}}{3} - 0.35 \right) \frac{\sqrt{\rho_L}}{\rho_L - \rho_g}$$

(6.10b)

$$Fr_d^h = 0.54 - \frac{N_f^{-1}}{1.886 + 0.01443 N_f^{-1}},$$

(6.10c)

$$Q = \begin{cases} c(\Delta Fr_d)^d \sin \theta (1 - \sin \theta), & \text{if } \Delta Fr_d \geq 0, \\ 0, & \text{if } \Delta Fr_d < 0. \end{cases}$$

(6.10d)

Other experimental studies of slug flow in slightly deviated from horizontal tubes have been carried out by Bonnecaze et al. (1971) and Stanislav et al. (1986). CFD simulations of Taylor bubbles in inclined pipes are computationally expensive, because axisymmetry cannot be assumed; as a result, there is no extensive study on the matter in the literature, and only Taha and Cui (2006) reported one inclined pipe case in their work.
As reviewed above, most multiphase models and correlations were developed with and for low viscosity fluids. For example, Bendiksen (1984) and Hasan and Kabir (1988a) used water, whose $Mo = 2.63 \cdot 10^{-11}$, a value which is within one order of magnitude of that for low viscosity oils. However, the oil and gas industry is currently moving towards the production of heavier oils. High density and high viscosity oils currently constitute nearly 70% of the available reserves in the world, increasing the need to gain and improve the knowledge of the flow behavior of these fluids. When $\mu \in [0.150, 1]$ Pa-s, oils are considered to be high viscous; medium viscosity oils when $\mu \in [0.030, 0.150]$ Pa-s; and low viscosity oils when $\mu \in [0.001, 0.030]$ Pa-s, corresponding to a $Mo$ range of $[1 \cdot 10^{-10}, 5 \cdot 10^3]$. Furthermore, the range of $Eo$ relevant to Taylor bubbles is $Eo \in [10, 700]$. Note that for $Eo \lesssim 4$ in vertical pipes, the bubble occupies the entire pipe cross section and basically does not move (White and Beardmore, 1962). On the other hand, Kataoka and Ishii (1987) proposed that the maximum stable cap bubble size for vertical pipes occurs at approximately $Eo \approx 900$, similar to what Kocamustafaogullari and Ishii (1985) predicted based on a two-dimensional Kelvin-Helmholtz instability analysis, and the experimental values reported by Clift et al. (2005). The implication is that the maximum pipe diameter for which Taylor bubbles and thus slug flow can exist corresponds to $Eo \approx 900$. In such pipes, bubbly flow transitions to either cap flow or churn-turbulent flow as the gas velocity increases (Cheng et al., 1998; Ohnuki and Akimoto, 2000; Prasser et al., 2005; Peng et al., 2010). It should be noted that this limit increases with increasing inclination angle, i.e. slug flow can exist in inclined pipes at larger diameters than in vertical pipes (Jepson and Taylor, 1993; Oddie et al., 2003). However, the critical values of the $Eo$ number at which this transition occurs are not available in the literature.
6.3 CMFD simulations

6.3.1 Mathematical model

3-D CFD simulations are performed with the CMFD code TransAT® (2014), a finite-volume software developed at ASCOMP. More details about the code can be found in chapter 4.

6.3.2 CMFD simulations

The text matrix explored in this study covers the ranges $Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^3]$ and $Eo \in [10, 700]$, and consists of the 25 logarithmically spaced cases shown in Figure 6-1 and summarized in Table 6.1. It can be observed that there are more points for lower $Eo$ as there is a sharp transition in the velocity behavior for $Eo \approx 15$, as shown later. For each case, up to seven inclination angles ($5°, 15°, 30°, 45°, 60°, 75°, 90°$) are simulated for a total of 147. This test matrix constitutes a substantial expansion of the ranges of parameters explored in previous studies.

The simulations start with a single bubble in still liquid and finish when the bubble reaches its terminal velocity. The bubble is placed inside a closed pipe embedded in the numerical domain (see figure 4-2 of section 4.2, chapter 4). The boundary conditions of the numerical domain are symmetry planes where the normal velocity and pressure gradient components are set to zero. The solid phase velocity is set to zero, and the no-slip condition at the wall is imposed through a relaxation term which acts as a distributed momentum sink reducing the fluid velocity as the indicator function goes to zero (Beckermann et al., 1999). The structured mesh size is dependent on the case study and is refined until the terminal velocity converges (see figure 4-3 of section 4.2, chapter 4). The mesh is locally refined next to the pipe walls. Number of cells ranges from 1 million up to 8.5 million cells.

Furthermore, two assumptions are made: the Taylor bubble length does not affect its rising velocity in inclined pipes and there exists a lubricating film between the Taylor bubble and the pipe wall at all inclinations. The first assumption is justified in section 5.3, chapter 5.
Figure 6-1: The map of White and Beardmore (1962) with the location of the numbered numerical database generated to obtain the Fr correlation of equations 6.15 (●), numerical cases used to validate the CMFD code (○, where □ are the experiments performed in this study), and experimental cases gathered from the literature (Zukoski, 1966; Weber et al., 1986; Shosho and Ryan, 2001; Gokcal et al., 2009b; Moreiras et al., 2014) to test the proposed correlation (×).
The second assumption is verified by application of the film drainage and breakup criterion proposed in Lizarraga-Garcia et al. (2016), described also in section 5.2, chapter 5. This criterion states that film breakup does not occur if the non-dimensional bubble passage time, $t_{\text{bubble}} = t_{\text{bubble}}/\tau < 0.01$, where $\tau$ is the characteristic drainage time. The bubble passage time can be calculated as $t_{\text{bubble}} = L/v$, where $L$ is the bubble length, and $v$ is the bubble velocity. The characteristic time is $\tau = 3\mu R/(2\rho g \cos \theta h_c^2)$, where $h_c$ is the critical thickness. The critical thickness order-of-magnitude estimate for the cases studied in steel pipe is $h_c \sim 1\mu m$, using the expressions of Vrij (1966). The most critical case we simulate is that for $\theta = 5^\circ$. At that point, the critical length below which the film does not break is calculated based on the aforementioned criterion as

$$\left( \frac{L}{d} \right)_c = \frac{v \tau 0.01}{d}. \quad (6.11)$$

The results from 6.11 are reported in the last column of table 6.2. The lowest value of $(L/d)_c$ is three hundred, that is, the length of the Taylor bubble simulated is much lower than the critical length calculated. Thus, the lubricating film is indeed present above the Taylor bubble in all cases simulated.

Representative snapshots of the shape and streamlines of a Taylor bubble with $Eo = 29$, $Mo = 0.07$, and $\theta = 30^\circ$ are shown in figure 6-2. We have validated the TransAT® code using data from the literature for the Taylor bubble terminal velocity, shape and velocity.
vectors in vertical and inclined pipes in chapter 4 (Lizarraga-Garcia et al., 2015b).

6.4 Results: Terminal velocity

For vertical pipes, the \( Fr \) obtained numerically with TransAT\(^\text{®} \) is compared with the results obtained using the correlations of Viana et al. (2003) and Kurimoto et al. (2013). The average terminal error of the simulations is 3.9% and 7.4%, with a standard deviation of 1.1% and 1.5%, respectively (see figure 6-3a). Based on this results, the correlation of Viana et al. (2003) appears to be an accurate tool to predict the terminal velocity of Taylor bubbles in vertical pipes. Furthermore, the film thickness, \( \bar{h} = h/d \), is compared with the correlation of Llewellin et al. (2012). Although the authors developed the correlation using experimental data where interfacial tension can be neglected, they proposed a generalization of the model to the cases where interfacial tension cannot be neglected. According to our data, this works well: the average error is 3.1%±1.3%.

![Figure 6-3: Taylor bubble terminal \( Fr \) (a) and \( \bar{h} = h/d \) (b) numerical results compared with the values obtained from literature correlations for vertical pipes](image)

As far as inclined pipes are concerned, figure 4-10 of chapter 4 shows the results from a few representative simulations of ours and the predictions of the correlations described above: Bendiksen (1984) (equations 6.4), Hasan and Kabir (1988a) (equations 6.6), Petalas
Table 6.2: Numerical database for the vertical pipe simulations

<table>
<thead>
<tr>
<th>Case</th>
<th>$E_o$</th>
<th>$M_o$</th>
<th>$N_f$</th>
<th>$F_r$</th>
<th>$(L/d)_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Simulations</td>
<td>Viana et al. (2003)</td>
</tr>
<tr>
<td>1</td>
<td>10</td>
<td>$1\cdot10^{-6}$</td>
<td>180</td>
<td>0.13</td>
<td>0.14</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td>$2.7\cdot10^{-4}$</td>
<td>44</td>
<td>0.063</td>
<td>0.066</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td>$7.1\cdot10^{-2}$</td>
<td>11</td>
<td>0.019</td>
<td>0.16</td>
</tr>
<tr>
<td>4</td>
<td>10</td>
<td>19</td>
<td>2.7</td>
<td>0.0038</td>
<td>0.0038</td>
</tr>
<tr>
<td>5</td>
<td>17</td>
<td>$1\cdot10^{-6}$</td>
<td>260</td>
<td>0.23</td>
<td>0.25</td>
</tr>
<tr>
<td>6</td>
<td>17</td>
<td>$2.7\cdot10^{-4}$</td>
<td>66</td>
<td>0.17</td>
<td>0.19</td>
</tr>
<tr>
<td>7</td>
<td>17</td>
<td>$7.1\cdot10^{-2}$</td>
<td>16</td>
<td>0.063</td>
<td>0.063</td>
</tr>
<tr>
<td>8</td>
<td>17</td>
<td>19</td>
<td>4.0</td>
<td>0.16</td>
<td>0.015</td>
</tr>
<tr>
<td>9</td>
<td>29</td>
<td>$1\cdot10^{-6}$</td>
<td>390</td>
<td>0.25</td>
<td>0.31</td>
</tr>
<tr>
<td>10</td>
<td>29</td>
<td>$2.7\cdot10^{-4}$</td>
<td>98</td>
<td>0.13</td>
<td>0.26</td>
</tr>
<tr>
<td>11</td>
<td>29</td>
<td>$7.1\cdot10^{-2}$</td>
<td>24</td>
<td>0.042</td>
<td>0.13</td>
</tr>
<tr>
<td>12</td>
<td>31</td>
<td>19</td>
<td>6.3</td>
<td>0.042</td>
<td>0.043</td>
</tr>
<tr>
<td>13</td>
<td>29</td>
<td>$5\cdot10^3$</td>
<td>1.5</td>
<td>0.0095</td>
<td>0.0095</td>
</tr>
<tr>
<td>14</td>
<td>84</td>
<td>$1\cdot10^{-6}$</td>
<td>870</td>
<td>0.34</td>
<td>0.34</td>
</tr>
<tr>
<td>15</td>
<td>84</td>
<td>$2.7\cdot10^{-4}$</td>
<td>220</td>
<td>0.30</td>
<td>0.32</td>
</tr>
<tr>
<td>16</td>
<td>84</td>
<td>$7.1\cdot10^{-2}$</td>
<td>54</td>
<td>0.25</td>
<td>0.25</td>
</tr>
<tr>
<td>17</td>
<td>84</td>
<td>19</td>
<td>13</td>
<td>0.11</td>
<td>0.11</td>
</tr>
<tr>
<td>18</td>
<td>84</td>
<td>$5\cdot10^3$</td>
<td>3.3</td>
<td>0.030</td>
<td>0.031</td>
</tr>
<tr>
<td>19</td>
<td>240</td>
<td>$1\cdot10^{-6}$</td>
<td>1900</td>
<td>0.36</td>
<td>0.34</td>
</tr>
<tr>
<td>20</td>
<td>240</td>
<td>$2.7\cdot10^{-4}$</td>
<td>480</td>
<td>0.34</td>
<td>0.34</td>
</tr>
<tr>
<td>21</td>
<td>240</td>
<td>$7.1\cdot10^{-2}$</td>
<td>120</td>
<td>0.31</td>
<td>0.31</td>
</tr>
<tr>
<td>22</td>
<td>240</td>
<td>19</td>
<td>30</td>
<td>0.21</td>
<td>0.20</td>
</tr>
<tr>
<td>23</td>
<td>240</td>
<td>$5\cdot10^3$</td>
<td>7.3</td>
<td>0.071</td>
<td>0.070</td>
</tr>
<tr>
<td>24</td>
<td>700</td>
<td>19</td>
<td>65</td>
<td>0.28</td>
<td>0.28</td>
</tr>
<tr>
<td>25</td>
<td>700</td>
<td>$5\cdot10^3$</td>
<td>16</td>
<td>0.15</td>
<td>0.14</td>
</tr>
</tbody>
</table>
and Aziz (2000) (equations 6.7), Gokcal et al. (2009b) (equations 6.8), Jeyachandra et al. (2012) (equations 6.9), and Moreiras et al. (2014) (equations 6.10). Note the agreement of the correlations with each other and the numerical data is rather poor, which further motivates the need for a new broadly-applicable and accurate correlation.

Our complete numerical database is shown in figure 6-4. The plots are superimposed over the $Eo - Mo$ map, and then within each plot the dependence of $Fr/Fr_v$ on the inclination angle is shown, where $Fr_v$ is the vertical pipe $Fr$. The continuous lines in the plots are from the models explained in the next section. For each case, the maximum value occurs at around $\theta = 45^\circ$ and results from the competing effects of drag coefficient (lower at lower angles, where most of the liquid “bypasses” the bubble through a larger flow area), and buoyancy (higher at higher angle). Furthermore, two distinct regions are observed regarding the maximum value of the normalized $Fr$, $(Fr/Fr_v)$: for $Eo > 20$, the amplitude of $Fr/Fr_v$ is small for low $Mo$ and high $Eo$, and slightly higher for high $Mo$--low $Eo$ cases. However, for $Eo < 20$, this amplitude is significantly bigger. At this $Eo$ range and vertical pipes, the bubble presents a bulge of higher radius in its bottom, making the liquid film effectively thinner and increasing the form drag. For example, the bulge can only be observed for the cases with $Eo = 10$ and 17 of figure 6-5, where the bubble bottom shape is shown for the cases with $\theta = 90^\circ$, and $Mo = 7.1 \cdot 10^{-2}$ and 19, respectively. As the pipe inclines, the bubble moves to the wall and the flow area increases in higher proportion than for the cases with $Eo > 20$, as the disappearance of the bulge also contributes to this increment. Another feature observed in the map is the flat profile for low $Mo$ and high $Eo$ cases, where the velocity drops rapidly for low inclination angles.

6.5 Proposed new correlation for Taylor bubble velocity

We will now use the numerical database to generate a correlation that can serve as closure relation for Taylor bubble velocity in mechanistic models of slug flow. Following the procedure of Hasan and Kabir (1988a), we can start by considering the balance of buoyancy and drag force that determines the terminal velocity of a Taylor bubble; after the $\tilde{p}$-groups
Figure 6-4: Normalized Taylor bubble terminal $Fr (Fr/F_{r_v})$, for the values of $Eo - Mo$ shown in figure 6-1: numerical results (o), correlation of equation 6.13 (---), and correlation of equations 6.15 (---).

Figure 6-5: Taylor bubble bottom shape for the cases with $\theta = 90^\circ$, and $Mo = 7.1 \cdot 10^{-2}$ (a) and 19 (b). The bulge at the bottom decreases with $Eo$ and disappears for $Eo > 20$.

are introduced, the force balance yields an expression for $Fr$ as follows:

$$\frac{Fr_0}{Fr_v} = (\sin \theta)^{1/2} g(Eo, Mo, \theta),$$

(6.12)
where the function \( g(E_o, M_o, \theta) \) is assumed to be \((1 + \cos \theta)^{E_o M_o^b}\) so that

\[
\frac{F_{r \theta}}{F_{r_v}} = (\sin \theta)^{1/2}(1 + \cos \theta)^{E_o M_o^b},
\]

(6.13)

and the exponents \( a \) and \( b \) are then fitted to maximize the accuracy of equation 6.13 in reproducing the numerical database. The fit is performed using the nonlinear optimization algorithms built in MATLAB® (2013). However, the results are not satisfactory at low inclination angles, and for high values of \( M_o \) and low values of \( E_o \) (see figure 6-4). Thus, a new function is proposed:

\[
Fr = F_{r_v}(1 - \exp(-b(E_o, M_o)\theta))(1 + c(E_o, M_o)\sin(2\theta)),
\]

(6.14)

where the exponential function reproduces the rapid velocity decay observed at low inclination angles, and the sinusoidal function reproduces the maximum velocity at \( \theta = 45^\circ \). The coefficients \( b(E_o, M_o) \) and \( c(E_o, M_o) \) are chosen to yield the most accurate fit:

\[
\begin{align*}
F_{r} &= F_{r_v}(1 - \exp(-b(E_o, M_o)\theta))(1 + c(E_o, M_o)\sin(2\theta)), \\
b(E_o, M_o) &= 47.06 F_{r_v} + 4, \\
c(E_o, M_o) &= -0.9118 F_{r_v} + 0.67 + \frac{(-0.0148 \log_{10} M_o)^2 + 0.125 \log_{10} M_o + 0.9118 F_{r_v} + 1.118}{(1 + (E_o/20)^8)^8}. 
\end{align*}
\]

(6.15a,b,c)

For the coefficient \( c(E_o, M_o) \), a logistic dose-response curve is used to connect the two differentiated regions described above (Patankar et al., 2002; Joseph and Yang, 2010). In order to use this new correlation for any values of \( E_o, M_o \) (or \( N_f \)) and \( \theta \), first calculate \( F_{r_v} \) from the correlation model of Viana et al. (2003), equations 6.3. Then, calculate the coefficients \( b \) and \( c \) from equations 6.15b and 6.15c, respectively, and finally, calculate \( Fr \) from equation 6.15a. Note that equation 6.15 is a continuous and smooth function of all the relevant variables and thus suitable for use as a closure relation in codes that implement the mechanistic model.
6.6 Performance of the new correlation

In this section, the performance of the proposed correlation (equations 6.15) is compared with the performance of the other correlations and models in the literature: Bendiksen (1984) (equations 6.4), Hasan and Kabir (1988a) (equations 6.6), Petalas and Aziz (2000) (equations 6.7), Gokcal et al. (2009b) (equations 6.8), Jeyachandra et al. (2012) (equations 6.9), and Moreiras et al. (2014) (equations 6.10). Two databases are used for the comparison: the numerical database (section 6.6.1) and the experimental database (section 6.6.2). In the comparison we shall use several statistical parameters that characterize the performance of the models. \( E_1 \) is the average relative error in percentage points,

\[
E_1 = \left( \frac{1}{N} \sum_{i}^{N} \frac{F_{\text{pred},i} - F_{\text{sim},i}}{F_{\text{sim},i}} \right) \cdot 100, \tag{6.16}
\]

where \( N \) is the number of points, \( F_{\text{pred},i} \) is the predicted \( Fr \) value of case \( i \) using a correlation, and \( F_{\text{sim},i} \) is the numerically obtained \( Fr \) value of case \( i \). \( E_2 \) is the absolute average relative error in percentage points,

\[
E_2 = \left( \frac{1}{N} \sum_{i}^{N} \frac{|F_{\text{pred},i} - F_{\text{sim},i}|}{F_{\text{sim},i}} \right) \cdot 100, \tag{6.17}
\]

\( E_3 \) is the standard deviation of the relative error in percentage points,

\[
E_3 = \sqrt{\frac{1}{N-1} \sum_{i}^{N} \left( \frac{F_{\text{pred},i} - F_{\text{sim},i}}{F_{\text{sim},i}} - \frac{E_1}{100} \right)^2} \cdot 100, \tag{6.18}
\]

\( E_4 \) is the average error in basis points,

\[
E_4 = \frac{1}{N} \sum_{i}^{N} (F_{\text{pred},i} - F_{\text{sim},i}), \tag{6.19}
\]
$E_5$ is the absolute average error in basis points,

$$E_5 = \frac{1}{N} \sum_{i} |F_{r_{\text{pred}},i} - F_{r_{\text{sim}},i}|,$$  \hspace{1cm} (6.20)

$E_6$ is the standard deviation of the absolute error in basis points,

$$E_6 = \sqrt{\frac{1}{N-1} \sum_{i} (F_{r_{\text{pred}},i} - F_{r_{\text{sim}},i} - E_4)^2},$$  \hspace{1cm} (6.21)

and finally, $R^2$ is the coefficient of determination, a number that indicates how well data fit a model,

$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}},$$  \hspace{1cm} (6.22)

where $SS_{\text{res}}$ is the sum of squares of the residuals, also called the residual sum of squares, and $SS_{\text{tot}}$ is the total sum of squares which is proportional to the variance of the data:

$$SS_{\text{res}} = \sum_{i} (F_{r_{\text{sim}},i} - F_{r_{\text{pred}},i})^2,$$  \hspace{1cm} (6.23a)

$$SS_{\text{tot}} = \sum_{i} (F_{r_{\text{sim}},i} - \bar{F}_{r_{\text{sim}}})^2,$$  \hspace{1cm} (6.23b)

where $\bar{F}_{r_{\text{sim}}}$ is the mean of the observed data, $\bar{F}_{r_{\text{sim}}} = \sum_i F_{r_{\text{sim}},i}/N$.

### 6.6.1 Numerical database

Table 6.3 summarizes the error statistics. Figure 6-6a reports the values of $F_r$ from the numerical simulations versus the predictions of equations 6.15. On its right, figure 6-6b shows the cumulative plot of the relative error, $E_2$ (equation 6.17), for the numerical database. It can be seen that the proposed correlation outperforms the other ones: using the proposed correlation, up to 70% of the cases show a relative error, $E_2$, of less than 10%. On the other hand, the other literature models predict less than 10% of the cases with a relative error, $E_2$, of less than 10%. On the other hand, the other literature models predict less than 10%
of the cases with a relative error, $E_2$, of less than 10%. Figure 6-7 reports the values of $Fr$ from the numerical simulations versus the predictions of the correlations from literature. In general, literature correlations overpredict $Fr$.

![Figure 6-6: Fr numerical values versus the predictions of the proposed correlation, equations 6.15 (a), and cumulative plot of the relative error, $E_2$, for the numerical database using the proposed and literature correlations (b).](image)

Of course the excellent performance of our correlation in reproducing the numerical database is not surprising since it was developed as a best fit of the numerical database, and the functions proposed are able to capture the velocity trends.

Table 6.3: Statistical parameters of the models analyzed using the numerical database generated

<table>
<thead>
<tr>
<th>Model</th>
<th>$E_1$</th>
<th>$E_2$</th>
<th>$E_3$</th>
<th>$E_4$</th>
<th>$E_5$</th>
<th>$E_6$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bendiksen (1984)</td>
<td>860</td>
<td>860</td>
<td>2400</td>
<td>0.34</td>
<td>0.34</td>
<td>0.16</td>
<td>-5.79</td>
</tr>
<tr>
<td>Moreiras et al. (2014)</td>
<td>430</td>
<td>450</td>
<td>1400</td>
<td>0.22</td>
<td>0.22</td>
<td>0.14</td>
<td>-2.22</td>
</tr>
<tr>
<td>Hasan and Kabir (1988a)</td>
<td>530</td>
<td>540</td>
<td>1300</td>
<td>0.22</td>
<td>0.23</td>
<td>0.16</td>
<td>-2.55</td>
</tr>
<tr>
<td>Jeyachandra et al. (2012)</td>
<td>120</td>
<td>130</td>
<td>250</td>
<td>0.10</td>
<td>0.11</td>
<td>0.092</td>
<td>0.086</td>
</tr>
<tr>
<td>Petalas and Aziz (2000)</td>
<td>120</td>
<td>120</td>
<td>190</td>
<td>0.096</td>
<td>0.097</td>
<td>0.060</td>
<td>0.40</td>
</tr>
<tr>
<td>Gokcal et al. (2009b)</td>
<td>220</td>
<td>220</td>
<td>310</td>
<td>0.21</td>
<td>0.21</td>
<td>0.10</td>
<td>-1.63</td>
</tr>
<tr>
<td>Proposed (equations 6.15)</td>
<td>1.4</td>
<td>8.6</td>
<td>12.1</td>
<td>0.0041</td>
<td>0.017</td>
<td>0.026</td>
<td>0.976</td>
</tr>
</tbody>
</table>
Figure 6-7: $Fr$ numerical values versus the predictions of the correlation of Bendiksen (1984) (equations 6.4) (a), Hasan and Kabir (1988a) (equations 6.6) (b), Petalas and Aziz (2000) (equations 6.7) (c), Gokcal et al. (2009b) (equations 6.8) (d), Jeyachandra et al. (2012) (equations 6.9) (e), and Moreiras et al. (2014) (equations 6.10) (f).
6.6.2 Experimental database

We have also tested the models against the experimental data shown in figure 6-8a, and reported in Appendix A. It is worth mentioning that these experimental data were not used in fitting the coefficients of equations 6.15. The 178 experimental datapoints, gathered from the literature (Zukoski, 1966; Weber et al., 1986; Shosho and Ryan, 2001; Gokcal et al., 2009b; Moreiras et al., 2014), cover the whole range of inclination angles and an ample region in the $Eo - Mo$ map. Figure 6-8b depicts the results of $Fr/Fr_v$ for both the experimental values and the predicted ones with equations 6.15. In general, the model predicts well the behavior except for cases 6 and 7, which were performed with an air/water mixture with $Mo = 2.63 \times 10^{-11}$ outside the ranges of our numerical database, as seen in figure 6-8a. Figure 6-10 reports the values of $Fr$ from the experiments versus the predictions of the correlations from literature. In general, literature correlations overpredict $Fr$, similarly to the numerical results above.

Figure 6-8: Numbered experimental cases gathered from the literature (Zukoski, 1966; Weber et al., 1986; Shosho and Ryan, 2001; Gokcal et al., 2009b; Moreiras et al., 2014) to test our model ($\times$) located in the map of White and Beardmore (1962) together with the numerical database developed in this study ($\bullet$) and the cases to validate the CMFD code ($\circ$, $\Box$) (a), and the Taylor bubble terminal $Fr$ over the vertical $Fr_v$, $Fr/Fr_v$, for the experimental database: experimental results ($\circ$), and predictions of equations 6.15 ($-$) (b).
Figure 6-9a depicts the experimental values of $Fr$ versus the proposed correlation. Furthermore, the cumulative error plot of the relative error, $E_2$, for the experimental database is shown in figure 6-9b. It can be seen that the proposed correlation again outperforms the other ones: using the proposed model, up to 70% of the cases show a relative error, $E_2$, of less than 10%. On the other hand, around 20% of the cases show a relative error, $E_2$, of less than 10% using the literature models. The three datapoints of figure 6-9a that are well below the 30% prediction error correspond to $\theta = 5^\circ$ of Shosho and Ryan (2001) (cases 18, 19 and 22 of figure 6-8b) where the velocity is remarkably low.

![Figure 6-9: Fr experimental values versus the predictions of the proposed correlation, equations 6.15 (a), and cumulative plot of the relative error, $E_2$, for the experimental database using the proposed and literature correlations (b).](image)

Finally, table 6.4 shows the statistical parameters that characterize the performance of the models. It is worth noting that our proposed correlation reports an $R^2 = 0.84$, while without the cases 6 and 7 $R^2 = 0.87$. The second best model is that of Jeyachandra et al. (2012) with $R^2 = 0.17$. Moreover, both $E_2$ and $E_3$ are 13% and 39% for our proposed model, respectively, while they are 37% and 56%, respectively, using the model of Jeyachandra et al. (2012).
Table 6.4: Statistical parameters of the models analyzed using the experimental database shown in figure 6-8a

<table>
<thead>
<tr>
<th>Model</th>
<th>$E_1$</th>
<th>$E_2$</th>
<th>$E_3$</th>
<th>$E_4$</th>
<th>$E_5$</th>
<th>$E_6$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bendiksen (1984)</td>
<td>110</td>
<td>110</td>
<td>190</td>
<td>0.20</td>
<td>0.20</td>
<td>0.13</td>
<td>-2.90</td>
</tr>
<tr>
<td>Moreiras et al. (2014)</td>
<td>63</td>
<td>64</td>
<td>130</td>
<td>0.12</td>
<td>0.13</td>
<td>0.10</td>
<td>-0.81</td>
</tr>
<tr>
<td>Hasan and Kabir (1988a)</td>
<td>66</td>
<td>69</td>
<td>130</td>
<td>0.11</td>
<td>0.12</td>
<td>0.12</td>
<td>-0.79</td>
</tr>
<tr>
<td>Jeyachandra et al. (2012)</td>
<td>34</td>
<td>37</td>
<td>56</td>
<td>0.087</td>
<td>0.095</td>
<td>0.068</td>
<td>0.17</td>
</tr>
<tr>
<td>Petalas and Aziz (2000)</td>
<td>35</td>
<td>39</td>
<td>65</td>
<td>0.080</td>
<td>0.093</td>
<td>0.087</td>
<td>0.052</td>
</tr>
<tr>
<td>Gokcal et al. (2009b)</td>
<td>51</td>
<td>52</td>
<td>94</td>
<td>0.12</td>
<td>0.13</td>
<td>0.083</td>
<td>-0.50</td>
</tr>
<tr>
<td>Proposed (equations 6.15)</td>
<td>0.32</td>
<td>13</td>
<td>39</td>
<td>-0.104</td>
<td>0.032</td>
<td>0.048</td>
<td>0.84</td>
</tr>
</tbody>
</table>
Figure 6-10: $Fr$ experimental values versus the predictions of Bendiksen (1984) (equations 6.4) (a), Hasan and Kabir (1988a) (equations 6.6) (b), Petalas and Aziz (2000) (equations 6.7) (c), Gokcal et al. (2009b) (equations 6.8) (d), Jeyachandra et al. (2012) (equations 6.9) (e), and Moreiras et al. (2014) (equations 6.10) (f).
6.7 Results: Hydrodynamic features

The 3D simulations provide plenty of information. Besides the terminal velocity, other interesting hydrodynamic characteristics are postprocessed. Figure 6-11 depicts the reported features in Taylor bubble in a vertical pipe (a), and in an inclined pipe (b): the film thickness, $h$; the perturbed distance upstream, $Z'$, and downstream, $L_{min}$, the bubble; the film developing length, $Z^*$, and the bubble tip position with respect to the centerline for inclined pipes, $y_{tip}$. The perturbed distances above and below the bubble, $Z'$ and $L_{min}$, respectively, are of particular importance in slug flow as they represent the area of influence of the Taylor bubble, which is relevant for coalescence phenomena in transient slug flow. The notation of these variables followed the one from Araújo et al. (2012), who reported different characteristics of individual Taylor bubbles rising in vertical pipes of stagnant liquids for an ample range of fluid properties and diameters ($Eo \in [6,900]$, $Mo \in [4.72 \cdot 10^{-5}, 104]$, $N_f \in [3.5,517]$). It should be noted that these values are later non-dimensionalized by the diameter of the pipe, $d$.

![Diagram](image_url)

Figure 6-11: Schematic of the hydrodynamic characteristics reported in this chapter.
6.7.1 Vertical pipe

The hydrodynamics characteristics of the vertical cases obtained numerically compare well with the correlations found in the literature. First, the dimensionless film thickness, $\tilde{h} = h/d$, is compared with the correlation of Llewellin et al. (2012). Its range of applicability is $10^{-1} < N_f < 10^5$ and $Eo > 40$, since they developed the correlation using experimental data where interfacial tension can be neglected. They also proposed a generalization of the model to the cases where interfacial tension cannot be neglected. According to our data, this generalization works well: the average error is $3.1\% \pm 1.3\%$ (Figure 6-3a). The cases with $Mo = 10^{-6}$ are slightly worse predicted, as the film thickness decreases more slowly with increasing $N_f$ than the trend obtained with the correlation of Llewellin et al. (2012).

Second, the dimensionless perturbed distance above the bubble, $Z'/d$, is depicted in figure 6-3b. This distance is determined by the point at the centerline in front of the bubble at which the vertical liquid velocity, $v_z$, is equal to 1% the value of $v_{TB}$, $v_z/v_{TB} = 0.01$. For lower $N_f$, $Z'/d$ is approximately constant and slightly higher than 0.483, the value reported by Araújo et al. (2012). As $N_f$ increases above 40 approximately, the perturbed distance increases as the lower viscosity means higher distance to diffuse the inertia. However, $Z'/d$ seems to reach a plateau at around 0.55, although more data at higher $N_f$ is needed to confirm this behavior. The dashed lines are the equations reported by Araújo et al. (2012), which follow well the reported results. It is worth noting that at approximately one radius ahead of the bubble, the liquid does not feel the presence of the bubble.

The third parameter reported for vertical pipes is the dimensionless film developing length, $Z^*/d$ (figure 6-3c). The criterion employed to obtain $Z^*/d$ is based on the two necessary conditions used by Araújo et al. (2012): the derivative of the vertical liquid film velocity, $v_z$, with respect to $z/d$ should be less than 5% of the maximum slope achieved along the developing film, and the radial component of the liquid film velocity, $v_r$, should be smaller than 5% the value of the maximum radial velocity obtained along the film, $v_{r,max}$. For $N_f < 100$, $Z^*/d$ presents a constant value slightly lower than 1, the value reported by Araújo et al. (2012). For $N_f > 100$, $Z^*/d$ increases because of the same reason as before:
lower viscosity means a higher distance to transfer the same momentum. However, the rate of increase observed is lower than the one reported by Araújo et al. (2012).

Finally, the dimensionless wake length, $L_{min}/d$, is analyzed in figure 6-3d. The criterion used to determine $L_{min}/d$ is the same as for $Z'/d$: the distance below the bubble at which the vertical liquid velocity, $v_z$, is equal to 1% the value of $v_{TB}$, $v_z/v_{TB} = 0.01$. Two important features can be inferred from figure 6-3d: the wake of the bubble, $L_{min}/d$, can reach much higher values than its influence above it, specially for lower $Mo$ numbers, and $L_{min}/d$ shows a higher dependence on $Eo$ and $Mo$ than $Z'/d$. The equations proposed by Araújo et al. (2012) work well for $Mo > 0.071$. However, for lower values of $Mo$ the behavior is not well captured. It should be noted that for some cases the $L_{min}/d$ reported is just a lower bound, as the pipe simulated was not long enough for the liquid below to reach the 1% the value of $v_{TB}$ in a region not affected by the pipe wall.

Furthermore, it is interesting to study when the tail of the bubble is concave or convex. Araújo et al. (2012) proposed a correlation for the transition based on data fitting dependent on $Eo$ and $Mo$:

$$\ln Eo = 4.305 + 0.087 \ln Mo. \quad (6.24)$$

Also, Lu and Prosperetti (2008) studied it based on physical phenomena. The authors claimed that the bubble tail is convex to the liquid or to the gas, for high or low surface tension, respectively. Thus, an approximate criterion for a convex bubble tail was formulated by observing that, for the tail to be convex, surface tension should be large enough to overcome the stagnant pressure below the tail. As the latter can be approximated by the dynamic pressure, the Weber number is obtained,

$$\text{We} = \frac{\rho L (v_{TB} - v_{SL})^2 d}{\sigma}, \quad (6.25)$$

where $v_{SL}$ is the superficial liquid velocity which is equal to zero, $v_{SL} = 0$, in a closed pipe. Thus, when $\text{We}$ is high, the stagnant pressure on the tail is high enough so that the tail is concave to the liquid. On the other hand, for low $\text{We}$, the surface tension force higher than
Figure 6-12: Vertical pipe hydrodynamic characteristics of the numerical database generated: dimensionless film thickness, $\bar{h} = h/d$, (a); dimensionless perturbed distance above the bubble, $Z'/d$, (b); dimensionless film developing length, $Z^*/d$, (c); and the dimensionless wake length, $L_{min}/d$ (d). Dashed lines on b, c, and d correspond to the correlations proposed by Araújo et al. (2012).
the stagnant pressure force and the tail is convex to the liquid. Based on their simulations, Lu and Prosperetti (2008) established the criterion at $We \approx 5$.

The numerical results of the current study compare well with both criteria. Figure 6-13a depicts the results by comparing with the criterion of Araújo et al. (2012), equation 6.24, and figure 6-13b shows the criterion of Lu and Prosperetti (2008), $We \approx 5$. Since some cases are difficult to classify as convex or concave since the tail is almost flat, a transition region is added to the figure 6-13b, i.e., when $We < 1.2$, the tail is convex to the liquid, and when $We > 5$, the tail is concave to the liquid:

\begin{align*}
\text{convex tail if } & We < 1.2, \\
\text{concave tail if } & We > 5.
\end{align*}

(6.26a) \hspace{1cm} (6.26b)

Figure 6-13: Reported convex tail to the liquid (o), concave tail to the liquid (x), and approximately flat tails (\(\triangledown\)) compared with the criterion from Araújo et al. (2012), equation 6.24 (a), and the criterion of Lu and Prosperetti (2008), $We \approx 5$ (b).
6.7.2 Inclined pipe

Similarly to the vertical pipe case, the hydrodynamic features highlighted in figure 6-11b can be extracted from the 3D CMFD simulations. In order to present the results, we make them dimensionless dividing either by the pipe diameter, \(d\), or by its value for the vertical case, shown before in figure 6-12.

Figure 6-14a depicts the film thickness over its vertical value, \(h/h_v\). It can be observed that those cases where the film thickness increases more pronouncedly with inclination angle at the beginning (cases 19, 14, 20), are those where the velocity profile is almost flat with inclination angle (see figure 6-4).

Figure 6-14b displays the bubble tip position with respect the centerline for inclined pipes over the pipe diameter, \(y_{tip}/d\). In general, the bubble tip of the cases with higher \(N_f\) located on the lower right part of the \(Eo - Mo\) map move more pronouncedly to the pipe wall as the pipe inclines than those with lower \(Eo\), whose bubble tip moves almost linearly to the pipe wall with \(\theta\).

Figure 6-14c depicts the perturbed distance above the bubble non-dimensionalized by the vertical pipe value, \(Z'/Z'_v\). In this case, this distance is determined by the cross section in front of the bubble at which the maximum liquid velocity component, \(v_{max} = \max(v_x, v_y, v_z)\), is equal to 1\% the value of \(v_{TB}\), \(v_{max}/v_{TB} = 0.01\). Its ranges lie within 1.5 and 2-times the value for the vertical case, i.e. around a diameter head of the bubble tip, and are not affected significantly by the inclination angle.

Figure 6-14d portrays the dimensionless film developing length, \(Z^*/Z^*_v\). The criterion to determine \(Z^*\) is the same as for the vertical case. It is interesting to note that while for the cases with lower \(Eo\) the developing length increases with lower \(\theta\), for mid-range \(Eo\) \(Z^*\) shows the opposite behavior. However, as seen above for \(Z'\), the inclination angle seems not to affect significantly the film developing length.

On the other hand, the wake length, \(L_{min}\), is the parameter most affected by the inclination angle, \(\theta\): for some cases, it increases several times the wake length of the vertical pipe case (see figure 6-14e).
Figure 6-14: Inclined pipe hydrodynamic characteristics of the numerical database generated: dimensionless film thickness, $h/h_v$, (a); dimensionless perturbed distance above the bubble, $Z'/Z_v^*$, (c); dimensionless film developing length, $Z^*/Z_v^*$, (d); dimensionless wake length, $L_{min}/L_{min,v}$, (e); and the symbols legend (f).
6.8 Conclusions

In this chapter, a new unified correlation for the terminal velocity of Taylor bubbles in pipes with a stagnant liquid for an ample range of fluid properties and pipe inclination angles was presented (equations 6.15). The correlation was developed based on a CMFD-generated database covering $Eo \in [10, 700]$, $Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^{3}]$, and $\theta \in [0^\circ, 90^\circ]$, and within those ranges it clearly outperforms current correlations when tested against both the numerical database and experimental data: the absolute average relative error is 8.6% and 13%, while the $R^2$ coefficient is 0.97 and 0.84, respectively. The second best correlation reports an absolute average relative error of 120% and 37%, and an $R^2$ coefficient of 0.40 and 0.17, respectively. The new correlation is recommended for use as a slug flow closure relation in codes that implement the mechanistic model. Furthermore, other interesting hydrodynamic features were presented. Furthermore, other hydrodynamic features were reported, of particular importance in slug flow the perturbed distances above and below the bubble, $Z'$ and $L_{\text{min}}$, respectively, as they represent the area of influence of the Taylor bubble, which is relevant for coalescence phenomena in transient slug flow. $Z'$ has been determined to not vary significantly with $Eo$, $Mo$ or $\theta$, as its maximum value is approximately $Z' \approx d$ for inclined pipes. On the other hand, the value of $L_{\text{min}}$ changes significantly with respect to the vertical pipe over the numerical database, and can reach up to 11 times that value for cases with $Mo = 5,000$. 
Chapter 7

Taylor Bubbles in Vertical and Inclined Pipes with Liquid Flow

7.1 Introduction

As introduced in the previous chapter, Taylor bubble velocity in two-phase flow is modeled based on the approach of Nicklin et al. (1962),

\[ v_{TB} = C_0 v_m + v_d, \]  

(7.1)

where \( v_d \) is the drift velocity of the bubble in stagnant liquid, and \( C_0 v_m \) is the contribution of the mixture velocity, \( v_m \), which is the sum of the liquid and gas superficial velocities, \( v_m = v_{SL} + v_{SG} \), respectively. \( C_0 \) is the distribution parameter which captures the effect of nonuniform flow and void concentration profiles.

Liquid flow adds a new parameter into the non-dimensional study of Taylor bubble’s dynamics. This is captured by the liquid flow Reynolds number, \( Re_{SL} = \rho_L v_{SL} d / \mu_L \). Thus, the Buckingham \( \pi \)-Theorem assures that the five \( \pi \)-groups are related by a unique function
\( Fr = f(Eo, Mo, Re_{SL}, \theta) \). In this chapter, we analyze this phenomenon through simulations of Taylor bubbles in upward and downward flow for the whole range of inclination angles. In particular, based on the model of Nicklin et al. (1962) (equation 7.1), we study the function \( C_0 \) such that

\[
F_{TB} = C_0(Eo, Mo, Re_{SL}, \theta) Fr_{SL} + Fr_d(Eo, Mo, \theta),
\]

(7.2)

where \( Fr_m = Fr_{SL} = \frac{v_{SL}}{\sqrt{gd}} \) since only liquid flows in the pipe. Note that \( Fr_d(Eo, Mo, \theta) \) is the correlation proposed in the previous chapter.

### 7.2 Literature review

Shortly after Nicklin et al. (1962), Zuber and Findlay (1965) proposed a general expression for two-phase flow systems that took into account both the effect of nonuniform flow and void concentration profiles as well as the effect of local relative velocity between the phases. The first effect was captured by the *distribution parameter*, \( C_0 \). The latter was accounted for by the weighted average drift velocity, which for Taylor bubbles is the drift velocity, \( v_d \).

Denoting by \( \langle F \rangle \) the average value of a quantity \( F \) over the cross-sectional area of the pipe,

\[
\langle F \rangle = \frac{1}{A} \int_A F dA,
\]

(7.3)

the expression derived therein is

\[
\bar{v}_g = C_0 \langle j \rangle + \frac{\langle \alpha v_g \rangle}{\langle \alpha \rangle},
\]

(7.4)

where \( \bar{v}_g \) is the *weighted average mean velocity* calculated as

\[
\bar{v}_g = \frac{\langle \alpha v_g \rangle}{\langle \alpha \rangle},
\]

(7.5)
\( \langle j \rangle \) is the average volumetric flux density of the mixture or mixture velocity \( v_m \), \( \alpha \) is the local void fraction, and \( v_{gj} \) is the drift velocity,

\[
v_{gj} = v_g - \dot{j}.
\] (7.6)

The effect of local relative velocity between the phases is captured by the second term of the RHS of equation 7.4. In slug flow, the local drift velocity is not affected by the concentration, thus

\[
\frac{\langle \alpha v_{gj} \rangle}{\langle \alpha \rangle} = v_{gj},
\] (7.7)

which is the previously named drift velocity of the Taylor bubble in stagnant liquid, \( v_d \). Thus, it can be seen that equation 7.1 is just the application of equation 7.4 for the Taylor bubble of slug flow so that \( \bar{v}_g = \bar{v}_{TB} \).

The distribution parameter \( C_0 \) is defined as

\[
C_0 = \frac{\langle \alpha v_m \rangle}{\langle \alpha \rangle \langle v_m \rangle},
\] (7.8)

already introduced in the equation 2.9 of section 2.4, chapter 2. In vertical slug flow, the Taylor bubble occupies almost the entire pipe thus \( \langle \alpha \rangle \approx 1 \). Furthermore, since the Taylor bubble occupies the center part of the pipe where the velocity is higher, \( C_0 > 1 \). However, Taitel and Barnea (1990) mentioned that “This factor \( [C_0] \) is influenced by the liquid velocity profile ahead of the bubble. This expression is very similar to the Zuber and Findlay (1965) distribution parameter, although here it results from an entirely different reason.” Currently, it does not exist a theoretical expression for \( C_0 \) but experimental correlations.

The literature for upward flow in vertical pipes is ample. Experiments (Nicklin et al., 1962; Bendiksen, 1985; Polonsky et al., 1999) and theory (Collins et al., 1978) have shown that \( C_0 \approx 2 \) for laminar flow and \( C_0 \approx 1.2 \) for turbulent flow are good engineering approximations for that case. Nicklin et al. (1962) measured Taylor bubble velocity for upward and downward water flow with liquid Reynolds number, \( Re_{SL} \), higher than 8,000. In their results, \( C_0 \approx 1.2 \) for upward flow. Bendiksen (1984) proposed that the previous engineer-
ing approximations are also applicable to upward inclined flow. An analytical investigation on $C_0$ for an axi-symmetrical bubble was performed by Collins et al. (1978) using inviscid theory.

Research on downward flow is more limited. Griffith and Wallis (1961) studied vertical upward and downward flow with air/water mixtures. Nicklin et al. (1962) reported that the situation is more complex in liquid downward flow because the rising bubble becomes non-axisymmetric. Martin (1976) performed experiments with air/water mixtures observing that only for small diameters ($Eo = 90$) the Taylor bubble remains eccentrically in the pipe axis. Consequently, the value of $C_0$ is lower. Bendiksen (1984) included $\theta = 0^\circ$ to $-30^\circ$ in his experiments. Roumazailles et al. (1996) performed experiments of downward turbulent slug flow with an air/kerosene mixture for inclination angles of $\theta = 0^\circ$ to $-30^\circ$, and claimed that the Taylor bubble velocity was not affected by the inclination angle in their experiments yielding $C_0 \approx 1.2$. Polonsky et al. (1999) analyzed the relation between the Taylor bubble velocity and the velocity field ahead of it through vertical upward and downward flows. They also reported tilting of the Taylor bubble tip towards the pipe wall in downward flow, and compared well the experimental coefficient $C_0$ with the liquid velocity at the bubble tip over the superficial liquid velocity, $v(tip)/v_{SL}$, in these cases.

Several experimental correlations for the distribution parameter, $C_0$, can be found in the literature. Bendiksen (1985) studied this parameter in vertical pipes, and proposed two different correlations for laminar and turbulent flow:

For laminar flow and $Eo > 40$,

$$
C_0 = 2.29 \left(1 - \frac{20}{Eo} \left(1 - e^{0.0125Eo}\right)\right),
$$

(7.9a)

For turbulent flow,

$$
C_0 = \frac{\log Re_{SL} + 0.309}{\log Re_{SL} - 0.743} \left(1 - \frac{2}{Eo} \left(3 - e^{-0.025Eo} \log Re_{SL}\right)\right),
$$

(7.9b)

where $Re_{SL}$ is the liquid flow Reynolds number, $Re_{SL} = \rho_L v_{SL} d/\mu_L$. Fréchou (1986) proposed a correlation dependent on $Re_{SL}$ only:

$$
C_0 = 1.2 + \frac{0.8}{1 + 1 \cdot 10^{-8} Re_{SL}^{2.55}}.
$$

(7.10)
Note that the previous equation cannot be applied for downward flow, \( \text{Re}_{SL} < 0 \). Also for vertical pipes, and based on air-water experiments, Tomiyama et al. (2001) proposed

\[
C_0 = \begin{cases} 
1.5 - 0.5e^{-4 \cdot 10^{-4} \text{Eo}^{2.36}}, & \text{for } \text{Re}_{SL} < 2,000, \\
1.18 + 0.32e^{1.7 \cdot 10^{-3} (2.300 - \text{Re}_{SL})}, & \text{for } \text{Re}_{SL} > 2,300.
\end{cases}
\]

Rattner and Garimella (2015) studied experimentally the intermediate scale Taylor flow, defined as \( 5 \leq \text{Eo} \leq 40 \), with air-water for \( 500 \leq \text{Re}_{SL} \leq 4.5 \cdot 10^3 \), and proposed a blended capillary-to-large scale distribution parameter, \( C_0 \), for this transitional regime with two contributions: the large scale, \( C_{0,LS} \), and the capillary scale, \( C_{0,Ca} \). The two contributions are blended with a large scale fraction function, \( f_{LS} \), as

\[
C_0 = f_{LS}C_{0,LS} + (1 - f_{LS})C_{0,Ca},
\]

where \( f_{LS} \) is equal to

\[
f_{LS} = \left( \frac{1}{1 + 4840 \text{Re}_{SL}^{-0.163}} \right)^{0.816/\text{Eo}}.
\]

The large scale contribution, \( C_{0,LS} \), is calculated as

\[
C_{0,LS} = 1.20 + \frac{1.09}{1 + (\text{Re}_{SL}/805)^4},
\]

and the capillary contribution, \( C_{0,Ca} \), is obtained from Liu et al. (2005):

\[
C_{0,Ca} = 1.20 + \frac{1.09}{1 + (\text{Re}_{SL}/805)^4}.
\]

This phenomenon has also been studied numerically. Mao and Dukler (1990, 1991) focused on the flow ahead and around the bubble. Hien and Fabre (2004b) provided analytical and numerical solutions for the velocity and shape of 2D long bubbles (plane and axisymmetric) for upward inclined flow. Taha and Cui (2006) simulated an air-water system with diameter \( d = 0.2 \text{m} \) (\( \text{Eo} = 55 \)). Lu and Prosperetti (2008) showed 2D axisymmetric simula-
tions in vertical pipes using VOF for $14.7 \leq Eo \leq 74.6$, $1.6 \cdot 10^{-11} \leq Mo \leq 1.6 \cdot 10^{-2}$, and $10 \leq Re_{SL} \leq 500$. Hua et al. (2012) used Fluent (VOF) to study water ($Mo = 2.54 \cdot 10^{-11}$) and SF$_6$ fluids in inclined pipes for $Eo = 1,350$ and $1 \cdot 10^4 \leq Re_{SL} \leq 3 \cdot 10^5$. For an inclination angle of $\theta = 5^\circ$, and after curve-fitting the data generated, they proposed that

$$v_{TB} = (0.863 + 0.0525v_m)v_m + 0.505\sqrt{gd},$$

(7.16)

i.e.,

$$C_0 = 0.863 + 0.0525v_m.$$

(7.17)

where the movement of the bubble nose towards the pipe centerline axis for higher flow rates explains the linear dependence of $C_0$ on $v_m$. Downward flow has not been studied with numerical simulations in the literature, to the best of our knowledge.

The only expression for $C_0$ for inclined upward flow found in the literature was that of Petalas and Aziz (2000), which depends on $Re_{SL}$ and $\theta$:

$$C_0 = (1.64 + 0.12 \sin \theta) Re_{SL}^{-0.031}.$$

(7.18)

Thus, the combined effect of the inclination angle, $\theta$, and $Eo$ on the distribution parameter, $C_0$, still needs to be further analyzed. Furthermore, the previous models and correlations were developed with and for low viscosity fluids, and the oil and gas industry is currently moving towards the production of heavier oils.

### 7.3 CMFD simulations

Here, we simulate individual Taylor bubbles with the fluid properties and pipe geometry corresponding to the three cases located in figure 7-1 (□) whose non-dimensional numbers are shown in table 7.1. These are based on the database generated for Taylor bubble in stagnant liquid described in the previous chapter, and are also spaced enough between each other so that they cover an ample range of fluid properties and pipe geometries. Results are
reported in the dimensionless form of equation 7.1, that is,

\[ Fr = C_0 Fr_{SL} + Fr_d. \]  

(7.19)

Note that the previous equation can also be presented using the liquid flow Reynolds number, \( Re_{SL} \), as

\[ Fr = C_0 \frac{Re_{SL}}{N_f} + Fr_d. \]  

(7.20)

For each case of figure 7-1, three different inclination angles \( \theta = 90^\circ, 45^\circ, 5^\circ \) are simulated. Moreover, Reynolds numbers studied are increased logarithmically \( (Re_{SL} = 1, 10, ...) \) until reaching the maximum \( Re_{SL} \) at which the Taylor bubble remains stable (see section 7.4.1). Furthermore, downward flow is also performed for each of the previous cases, that is, \( Re_{SL} = -1, -10, \) etc. A total of 40 cases are simulated.

The simulations start with a single bubble in still liquid and finish when the bubble reaches its terminal velocity, similar to the simulations of bubbles in stagnant liquid. The bubble is placed inside a pipe with both ends open and embedded in the numerical domain. The boundary conditions of the numerical domain are an inflow plane at the pipe inlet where the velocity is set to a transient profile that evolves from zero at the simulation start to the Hagen-Poiseuille profile, an outflow plane at the pipe outlet where the stream-wise gradients of all variables are set to zero (fully developed flow condition) and overall mass conservation is ensured, and finally symmetry planes at the other four planes parallel to the pipe longitudinal axis where the normal velocity and pressure gradient components are set to zero. The no-slip condition at the wall is imposed through a relaxation term which acts as a distributed momentum sink reducing the fluid velocity as the indicator function goes to zero (Beckermann et al., 1999). The structured mesh size is dependent on the case study and is refined until the terminal velocity converges. Number of cells ranges from 1 million up to 3.7 million cells.
Table 7.1: Test matrix for simulations of Taylor bubble motion in pipes with liquid flow

<table>
<thead>
<tr>
<th>Case</th>
<th>$E_0$</th>
<th>$M_0$</th>
<th>$N_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>29</td>
<td>7.1\times 10^{-2}</td>
<td>24</td>
</tr>
<tr>
<td>2</td>
<td>240</td>
<td>7.1\times 10^{-2}</td>
<td>120</td>
</tr>
<tr>
<td>3</td>
<td>700</td>
<td>5\times 10^3</td>
<td>16</td>
</tr>
</tbody>
</table>

Figure 7-1: Location in the map of White and Beardmore (1962) of the numbered numerical cases with imposed liquid flow (□), database generated for Taylor bubbles in stagnant liquid (●), and cases used to validate the CMFD code (○, □).

7.4 Results: Terminal velocity

In this section, we first analyze the results for vertical pipes, comparing the numerical results with the experimental correlations introduced before: $C_0 = 2$, Bendiksen (1985) (equation 7.9a), Fréchou (1986) (equation 7.10), Petalas and Aziz (2000) (equation 7.18),
and Tomiyama et al. (2001) (equation 7.11a). Note that the correlation of Fréchou (1986) and Petalas and Aziz (2000) cannot predict real $C_0$ for downward flow.

For upward flow in vertical pipes, results are similar in the three cases: bubble velocity is predicted well with equation 7.2 and $C_0 = 2$, and the bubble shape becomes more pointed as the liquid velocity increases. However, for downward flow results differ. For case 1, the bubble remains axisymmetric as the liquid flow increases in absolute value following the line obtained with $C_0 = 2$ ($Fr_{SL} < 0, Re_{SL} < 0$ in figure 7-2). For $Re_{SL} = -10$, the bubble moves downward in the pipe ($Fr < 0$) with the bubble tip pointing also downward. Figure 7-2a shows that the assumption of $C_0 = 2$ as well as the correlation of Fréchou (1986) work well in this case. For case 2, Taylor bubble shows a similar behavior as before besides when the liquid velocity is $Re_{SL} = -41$: there the bubble becomes non-axisymmetric (figure 7-3b) which strongly reduces the bubble drag coefficient and the bubble moves upward in the pipe ($Fr > 0$) despite the significant downward flow. In this case, experimental correlations overpredict $C_0$, whose value based on our numerical results is $C_0 = 0.72$. It is worth noting that case 1 and 2 only differ in their $Eo$: surface tension is less important in case 2 with respect to gravity and thus the bubble deforms and moves to the pipe wall, as opposed to the axisymmetric bubble of case 1. Furthermore, the bubble shape for $Re_{SL} = -41$ shown in figure 7-3b is obtained for different initial conditions. Finally, the behavior obtained with case 3 is similar to that of case 2, with the bubble becoming non-axisymmetric with lower Reynolds number as $Eo$ is higher: $Re_{SL} = -1$, figure 7-4. Numerical $C_0 = 1.32$ in this case.

For inclined pipes, the $C_0$ obtained based on the numerical results is typically lower than 2. For example, figure 7-5 depicts the Taylor bubble terminal $Fr$ versus $Fr_{SL}$ calculated numerically for 45° and 5° compared with the assumption of $C_0 = 2$ and the experimental correlation of Petalas and Aziz (2000) (equation 7.18). Again, note that the correlation of Petalas and Aziz (2000) cannot predict real $C_0$ for downward flow. Figure 7-6 shows the overall results for the cases shown in figure 7-1 compared with the equation 7.2 with $C_0 = 2$, where the horizontal dotted line delimits the upward and downward movement of the bubble.
Figure 7-2: Case 1 Taylor bubble terminal $Fr$ versus $Fr_{SL}$ calculated numerically compared with the experimental correlations for $\theta = 90^\circ$ (a), and bubble shapes for each of them (b).

Figure 7-3: Case 2 Taylor bubble terminal $Fr$ versus $Fr_{SL}$ calculated numerically compared with the experimental correlations for $\theta = 90^\circ$ (a), and bubble shapes for each of them (b).
Figure 7-4: Case 3 Taylor bubble terminal $Fr$ versus $Fr_{SL}$ calculated numerically compared with the experimental correlations for $\theta = 90^\circ$ (a), and bubble shapes for each of them (b).

Figure 7-5: Case 2 Taylor bubble terminal $Fr$ versus $Fr_{SL}$ calculated numerically compared with the experimental correlations for $\theta = 45^\circ$ (a) and $\theta = 5^\circ$ (b).
7.4.1 Critical upper Weber number, $W_{ec}$

As the liquid flow increases, the tail concavity to the liquid increases reaching a liquid flow value where the stagnant pressure on the bubble tail is so high that the surface tension cannot sustain it and a liquid jet breaks the bubble from below. Figure 7-7 shows this behavior for case 1 and 3. Figure 7-7a depicts case 1, where the dash-dotted line for $Re_{SL} = 100$ is an unstable cap bubble. On its right, the dash-dotted line for $Re_{SL} = 10$ is the unstable bubble for case 3, where the jet below the bubble is penetrating it. Here, we analyze the Weber number introduced in equation 6.25 of the previous chapter which determined the
Figure 7-7: Bubble tail shape for upward vertical flow of case 1 (a) and case 3 (b) for different flow velocities: the tail concavity to the liquid increases with increasing $We$.

tail convexity for Taylor bubbles in stagnant liquids:

$$We = \frac{\rho_L (v_{TB} - v_{SL})^2 d}{\sigma} = E_0 (Fr - Fr_{SL})^2. \quad (7.21)$$

In the current simulations, we have observed that the bubble becomes unstable for $We > 75$, although more simulations and experiments are needed to obtain a the critical Weber number $We_c$. Given a critical Weber value $We_c$, equation 7.21 can be solved to obtain an approximate $Fr_{SL}$ at which this occurs since $Fr = C_0 Fr_{SL} + Fr_d$ and assuming $C_0 = 2$ for laminar flow and $Fr_d$ from the the correlation of Viana et al. (2003). This value would set the upper $Re_{SL}$ simulated for each case.

### 7.5 Performance of the correlations for the terminal velocity

The statistical parameters introduced in section 6.6 of the previous chapter are also applied here. Table 7.2 reports the values for the vertical cases, table 7.3 reports those for $\theta = 45^\circ$, and table 7.4 for $\theta = 5^\circ$. The correlations of Fréchou (1986) and Petalas and
Aziz (2000) report good statistical parameters, although it is worth reminding that since those correlations cannot predict values for downward flow, these cases are not used in the parameter computation. In fact, the correlation of Fréchou (1986) provides a $C_0 \approx 2$ for the cases studied, so the differences in the parameters of $C_0 = 2$ and Fréchou (1986) of table 7.2 tell us that the approximation of $C_0 = 2$ is not as good for downward flow as for upward vertical pipes. $C_0$ obtained using the correlation of Petalas and Aziz (2000) provides ranges from 1.6 to 1.75 at $\theta = 45^\circ$ and from 1.55 to 1.65 at $\theta = 5^\circ$, thus the differences in tables 7.3 and 7.4 provide similar information as before. It is remarkable that this performance is much worse for cases at $\theta = 5^\circ$.

Table 7.2: Statistical parameters of the models analyzed using the numerical cases simulated (figure 7-6) for $\theta = 90^\circ$

<table>
<thead>
<tr>
<th>Model</th>
<th>$E_1$</th>
<th>$E_2$</th>
<th>$E_3$</th>
<th>$E_4$</th>
<th>$E_5$</th>
<th>$E_6$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_0 = 2$</td>
<td>-61.33</td>
<td>66.33</td>
<td>190.33</td>
<td>-0.064</td>
<td>0.068</td>
<td>0.13</td>
<td>0.93</td>
</tr>
<tr>
<td>Fréchou (1986)</td>
<td>-3.8</td>
<td>4.6</td>
<td>5.1</td>
<td>-0.036</td>
<td>0.040</td>
<td>0.064</td>
<td>0.98</td>
</tr>
<tr>
<td>Petalas and Aziz (2000)</td>
<td>-12.0</td>
<td>12.0</td>
<td>9.1</td>
<td>-0.11</td>
<td>0.11</td>
<td>0.15</td>
<td>0.87</td>
</tr>
<tr>
<td>Tomiyama et al. (2001)</td>
<td>-15.0</td>
<td>44.0</td>
<td>62.0</td>
<td>-0.061</td>
<td>0.14</td>
<td>0.22</td>
<td>0.82</td>
</tr>
<tr>
<td>Bendiksen (1985)</td>
<td>-3.7x10$^{25}$</td>
<td>1.7x10$^{26}$</td>
<td>4.0x10$^{26}$</td>
<td>6.6x10$^{23}$</td>
<td>7.9x10$^{23}$</td>
<td>2.3x10$^{24}$</td>
<td>-2.0x10$^{49}$</td>
</tr>
</tbody>
</table>

Table 7.3: Statistical parameters of the models analyzed using the numerical cases simulated (figure 7-6) for $\theta = 45^\circ$

<table>
<thead>
<tr>
<th>Model</th>
<th>$E_1$</th>
<th>$E_2$</th>
<th>$E_3$</th>
<th>$E_4$</th>
<th>$E_5$</th>
<th>$E_6$</th>
<th>$R^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_0 = 2$</td>
<td>5.4</td>
<td>19.0</td>
<td>29.0</td>
<td>-0.021</td>
<td>0.063</td>
<td>0.10</td>
<td>0.90</td>
</tr>
<tr>
<td>Petalas and Aziz (2000)</td>
<td>-0.60</td>
<td>7.0</td>
<td>8.9</td>
<td>-0.0041</td>
<td>0.032</td>
<td>0.048</td>
<td>0.98</td>
</tr>
</tbody>
</table>

7.6 Results: Hydrodynamic features

Here, we report the hydrodynamic characteristics sketched in figures 6-11 of section 6.8, chapter 6. Figure 7-8 depicts the non-dimensional film thickness, $h/d$, for each case and
Table 7.4: Statistical parameters of the models analyzed using the numerical cases simulated (figure 7-6) for \( \theta = 5^\circ \)

<table>
<thead>
<tr>
<th>Model</th>
<th>( E_1 )</th>
<th>( E_2 )</th>
<th>( E_3 )</th>
<th>( E_4 )</th>
<th>( E_5 )</th>
<th>( E_6 )</th>
<th>( R^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_0 = 2 )</td>
<td>500</td>
<td>510</td>
<td>1100</td>
<td>-0.017</td>
<td>0.063</td>
<td>0.11</td>
<td>0.92</td>
</tr>
<tr>
<td>Petalas and Aziz (2000)</td>
<td>1.1</td>
<td>6.7</td>
<td>9.1</td>
<td>-0.0070</td>
<td>0.035</td>
<td>0.057</td>
<td>0.96</td>
</tr>
</tbody>
</table>

Inclination angle. For the vertical cases \( \theta = 90^\circ \), the film thickness increases with liquid flow, but for the cases which become non-axisymmetric (see figures 7-3b and 7-4b before). For inclined pipes, the behavior is the opposite: film thickness increases with liquid flow, that is, the bubble moves closer to the wall and thins itself. The exception for this trend is for case 1, \( \theta = 5^\circ \), where the bubble moves downward in the pipe and moves closer to the centerline.

Figure 7-9 shows the bubble tip position with respect to the centerline, \( y_{tip}/d \), for each case and inclination angle. For the vertical cases \( \theta = 90^\circ \), the bubble tip remains in the centerline for the axisymmetric cases, and moves close to the wall when the bubble becomes non-axisymmetric. For inclined pipes, the bubble tends to move to the centerline as the liquid flow increases. For case 1 at \( Re_{SL} = -10 \) where the bubble moves downward the situation changes:: the bubble moves to the centerline.
Figure 7-8: Taylor bubble dimensionless film thickness, $h/d$, versus $Fr_{SL}$ for the cases shown in figure 7-1
Figure 7-9: Taylor bubble dimensionless tip position with respect to the centerline, $y_{tip}/d$, versus $Fr_{SL}$ for the cases shown in figure 7-1.
7.7 Conclusions

In this chapter, simulations of Taylor bubbles in inclined pipes with upward and downward flow were performed. As of now, a model with $C_0 = 2$ in equation 7.1 seems to behave the best for upward flow. However, for downward flow the bubble terminal velocity is ill-predicted by this assumption as the opposite flow modifies the bubble shape differently from the upward cases. In particular, Taylor bubble becomes non-axisymmetric beyond certain liquid flow values in vertical pipes. The liquid flow velocity at which this occurs lowers with increasing $Eo$. In fact, this behavior was not observed for $Eo = 29$, the lowest $Eo$ simulated. More cases should be completed in order to extract more conclusive information about these phenomena. Furthermore, a Taylor bubble breakup mechanism for lower than expected $Fr_{SL}$ was observed, where a liquid jet penetrates the bubble from its bottom.
Chapter 8

Conclusions and Future Work

The main objective of this work was to improve the prediction tools for two-phase slug flow in pipes through the use of multiphase CFD. In particular, the improvement of the so-called closure relations of the mechanistic models, correlations hitherto obtained empirically and that carried the highest uncertainties in these models.

First, we determined the dominant closure relations with respect to the models’ figures of merit, the void fraction (or liquid holdup) and the pressure drop, through sensitivity analysis of three different models (Orell and Rembrand, 1986; Ansari et al., 1994; Petalas and Aziz, 2000) in chapter 3. There, it was concluded that the Taylor bubble velocity, $v_{TB}$, affected significantly those figures of merit, thus we focused on the study of Taylor bubble’s dynamics from then on. The finite-volume CMFD code used in this study, Transat®, was validated with a series of Taylor bubble test cases described in chapter 4, which built enough confidence on the CMFD code to employ it to develop a new and broad numerical database from which one can study the dynamics of Taylor bubbles in inclined pipes. However, two main assumptions were made in the numerical simulations: (i) a lubricating film exists between the Taylor bubble and the pipe wall at all inclinations, and (ii) the Taylor bubble length does not affect its dynamics in inclined pipes. To verify the robustness of the first
assumption, an analytical model predicting the gravity-induced drainage of the thin film was presented in section 5.2, chapter 5, and from it, a new criterion to avoid the film breakup was derived: 
\[ \tilde{t}_{\text{bubble}} = \frac{t_{\text{bubble}}}{\tau} < 0.01, \]
where \( t_{\text{bubble}} \) is the Taylor bubble’s passage time and \( \tau \) is the characteristic drainage time. The model was experimentally validated through Taylor bubbles in inclined pipes with stagnant liquids (Lizarraga-Garcia et al., 2016). The second assumption was justified in section 5.3, chapter 5, through experiments performed in the laboratory and simulations.

In the literature, the Taylor bubble velocity is modeled based on two different contributions: (i) the drift velocity, i.e., the velocity of propagation of a Taylor bubble in stagnant liquid, and (ii) the liquid flow contribution. Here, we first analyzed the dynamics of Taylor bubbles in stagnant liquid by generating a large numerical database that covers the most ample range of fluid properties and pipe inclination angles explored to date: \( Eo \in [10, 700], Mo \in [1 \cdot 10^{-6}, 5 \cdot 10^3], \) and \( \theta \in [0^\circ, 90^\circ] \). A new unified Taylor bubble velocity correlation, proposed for use as a slug flow closure relation in the mechanistic model, was derived from that database employing logistic dose-response curves (equations 6.15). The new correlation clearly outperformed current correlations when tested against both the numerical database and experimental data: the absolute average relative error is 8.6% and 13.0%, while the coefficient of determination \( R^2 \) is 0.97 and 0.84, respectively. The second best correlation reported absolute average relative errors of 120% and 37%, and \( R^2 = 0.40 \) and 0.17, respectively. Furthermore, other hydrodynamic features were reported in section 6.7, chapter 6. Of particular importance in slug flow are the perturbed distances upstream and downstream the bubble, \( Z' \) and \( L_{\text{min}} \), respectively, as they represent the area of influence of the Taylor bubble, which is relevant for coalescence phenomena in transient slug flow. \( Z' \) was determined to not vary significantly with \( Eo, Mo \) or \( \theta \), as its maximum value is approximately \( Z' \approx d \) for inclined pipes. On the other hand, the value of \( L_{\text{min}} \) changed significantly with respect to the vertical pipe over the numerical database, and can reach up to 11 times that value for cases with \( Mo = 5,000 \).

Finally, simulations of Taylor bubbles in inclined pipes with upward and downward flow
were performed in chapter 7. As of now, a model with $C_0 = 2$ in the model of Nicklin et al. (1962) (equation 7.1) seems to behave the best for upward flow. However, for downward flow the bubble terminal velocity is ill-predicted by this approximation, specially when Taylor bubbles become non-axisymmetric beyond certain liquid flow values in vertical pipes. Furthermore, a Taylor bubble breakup mechanism for lower than expected liquid velocities was observed, where a liquid jet penetrates the bubble from its bottom.

Other important questions are still open. First, the bubble volume beyond which the bubble becomes a Taylor bubble. Based on our simulations, the volume needed to obtain a bubble terminal velocity independent of the volume itself increases with decreasing inclination angle with respect to the horizontal, $\theta$. Furthermore, it is still unknown the maximum $E_0$ at which Taylor bubbles exist in inclined pipes. Similarly to the previous trend, this critical $E_0$ increases as $\theta$ decreases. Another instability mechanism that still needs to be further evaluated is the breakup mechanism observed in Taylor bubbles in vertical pipes with liquid flow where the Taylor bubble bottom cannot sustain the stagnant pressure built on it and a liquid jet breaks it. We think that this breakup mechanism is captured by the Weber number defined in equation 7.21.

As a final remark, we have proven in this work that computational fluid dynamics are a useful and complementary resource to study slug flow and improve the current two-phase flow prediction tools. Future work could focus on other closure relations, such as the liquid slug void fraction, in order to deeper our understanding and obtain more accurate closure relations, or even on different flow regimes altogether.
## Appendix A

### Experimental database

Table A.1: Experimental database used in section 6.6.2, chapter 6

<table>
<thead>
<tr>
<th>Source</th>
<th>Liquid</th>
<th>$\rho_L$ [kg/m$^3$]</th>
<th>$\rho_g$ [kg/m$^3$]</th>
<th>$\mu_L$ [Pa·s]</th>
<th>$\sigma$ [N/m]</th>
<th>$d$ [m]</th>
<th>$\theta$ [$^\circ$]</th>
<th>$v_{TB}$ [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zukoski (1966)</td>
<td>Water</td>
<td>1000</td>
<td>1.8</td>
<td>0.001</td>
<td>0.072</td>
<td>0.0549</td>
<td>10</td>
<td>0.3818</td>
</tr>
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<td>0.0549</td>
<td>20</td>
<td>0.4017</td>
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<td>30</td>
<td>0.4178</td>
</tr>
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<td>0.0791</td>
<td>0.0373</td>
<td>90</td>
<td>0.1990</td>
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</tbody>
</table>
Table A.2: Experimental database used in section 6.6.2, chapter 6 (continuation)

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<th>Source</th>
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<th>( \rho_g ) [kg/m(^3)]</th>
<th>( \mu_L ) [Pa-s]</th>
<th>( \sigma ) [N/m]</th>
<th>( d ) [m]</th>
<th>( \theta ) [(^\circ)]</th>
<th>( v_{TB} ) [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
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<td>Sucrose</td>
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<td>1.8</td>
<td>0.518</td>
<td>0.079</td>
<td>0.0373</td>
<td>15</td>
<td>0.1808</td>
</tr>
<tr>
<td></td>
<td>Sucrose</td>
<td>1320</td>
<td>1.8</td>
<td>0.518</td>
<td>0.079</td>
<td>0.0373</td>
<td>30</td>
<td>0.2044</td>
</tr>
<tr>
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<td>Sucrose</td>
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<td>1.8</td>
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<td>Hybrid Linear/Parabolic Approximation</td>
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<td>Level Set</td>
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<td>MPI</td>
<td>Message Passing Interface</td>
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<td>ODE</td>
<td>Ordinary Differential Equation</td>
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<tr>
<td>PETSc</td>
<td>Portable, Extensible Toolkit for Scientific Computation</td>
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<td>PIV</td>
<td>Particle Image Velocimetry</td>
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<td>PWR</td>
<td>Pressure Water Reactor</td>
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<td>RHS</td>
<td>Right Hand Side</td>
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SIMPLEC  Semi-Implicit Method for Pressure Linked Equations-Consistent
SIP  Strongly Implicit Procedure
TUALP  Tulsa University Artificial Lift Projects
TUFFP  Tulsa University Fluid Flow Projects
VLE  Vapor/Liquid Equilibrium
VOF  Volume of Fluid

**Dimensionless Numbers**

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<td>((\rho_L - \rho_g) gd^2 / \sigma)</td>
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<tr>
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<td>Eötvös</td>
<td>(\rho_L gd^2 / \sigma)</td>
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<td>Eo_film</td>
<td>Film Eötvös</td>
<td>(\rho_L gh / \sigma \kappa)</td>
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<td>Fr</td>
<td>Froude</td>
<td>(v_{TB} / \sqrt{gd})</td>
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<tr>
<td>Mo</td>
<td>Morton</td>
<td>(g \mu_L^4 / \rho_L \sigma^3)</td>
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<td>NB</td>
<td>–</td>
<td>(\mu_L^2 v_s^2 \rho_g / \sigma^2 \rho_L)</td>
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<td>Nf</td>
<td>Inverse viscosity</td>
<td>(\rho_L (gd)^{1/2} d / \mu_L)</td>
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<td>Re</td>
<td>Reynolds</td>
<td>(\rho_L v_d / \mu_L)</td>
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<tr>
<td>We</td>
<td>Weber</td>
<td>(\rho_L (v_{TB} - v_{SL})^2 d / \sigma)</td>
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**Greek Symbols**

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<thead>
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<td>Viscosity</td>
<td>M/LT</td>
<td>Pa-s</td>
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<tr>
<td>$\overline{\sigma}$</td>
<td>Viscous stress tensor</td>
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<td>Intermolecular potential function in the liquid</td>
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<td>$\Pi$</td>
<td>Disjoining pressure</td>
<td>M/LT^2</td>
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</table>
\( \psi_d \) Deposition mass-transfer rate per unit volume \( \text{M/TL}^3 \) \( \text{kg/s·m}^3 \)

\( \psi_e \) Entrainment mass-transfer rate per unit volume \( \text{M/TL}^3 \) \( \text{kg/s·m}^3 \)

\( \psi_g \) Mass-transfer rate per unit volume between liquid and gas phases \( \text{M/TL}^3 \) \( \text{kg/s·m}^3 \)

\( \rho \) Density \( \text{M/L}^3 \) \( \text{kg/m}^3 \)

\( \sigma \) Standard deviation of the velocity \( \text{L/T} \) \( \text{m/s} \)

\( \sigma \) Surface tension \( \text{M/T}^2 \) \( \text{N/m} \)

\( \tau \) Drainage characteristic time \( \text{T} \) \( \text{s} \)

\( \tau_{wL} \) Wall shear stress \( \text{M/LT}^2 \) \( \text{Pa} \)

\( \theta \) Inclination angle with respect to the horizontal \( - \) \( - \) \( ° \)

\( \zeta \) Exponential coefficient \( - \) \( 1 \)

**Superscripts**

**Symbol** **Description**

h Horizontal

v Vertical

**Roman Symbols**

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<td>( \bar{t} )</td>
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<td>Hamaker constant</td>
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<td>Pipe cross-sectional area</td>
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<td>m²</td>
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<td>Specific internal energy</td>
<td>L²/T²</td>
<td>J/kg</td>
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<td>Average relative error in percentage points</td>
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<td>M/L(^2)T(^2) N/m(^3)</td>
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### Subscripts

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<td>SU</td>
<td>Slug unit</td>
</tr>
<tr>
<td>TB</td>
<td>Taylor bubble</td>
</tr>
</tbody>
</table>
tip        Taylor bubble tip
vdW        Van-der-Waals
Bibliography


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