Chapter 3: State of the art, simulation approaches.

3.1 Introduction:

This chapter treats the state of the art in the modeling of two phase flows, commenting the main differences among the approaches and the recent efforts in the modeling within the two fluids model.

In the CFD simulations of gas-liquid flows there are three basic numerical methods discussed in the literature that differ in the scale range that is explicitly solved.

- Direct Numerical Simulation (DNS), or interface resolving method: is at the lowest level of time and length scale. It aims to resolve all interactions between two phases and needs no turbulence and interfacial exchange models. Its main difficulty is the highest computational load, and as a result numerical methods of this type have been applied mostly to flows around a single bubble or to systems involving only a relatively small number of bubbles or particles. Another difficulty is the moving phase-interface whose shape is a part of the solution. To keep the interface numerically sharp special numerical algorithms have to be developed. Nowadays mainly three types of methods are used, the volume of-fluid method (VOF), the level-set method (LS) and the front-tracking (FT) method [Wieringa et al(1996)].

- Euler-Lagrange (E-L): For systems at intermediate scale, E-L or discrete bubble approach can be used where the liquid phase is solved by phase-averaged equations while bubbles are modeled by point force distributions at the discrete location of bubbles and the equation of motion is solved by Newton’s second law. Particularly suited to study the effect of bubble and/or bubble-wall interactions, contrary to the DNS approach, the flow field at the scale of an individual bubble is not resolved, and therefore closure laws for bubble-liquid interaction [Kawamura et al (2002)]. Its major disadvantage approach is the complexity of the interfacial coupling, since the coupling between two different solvers, i.e. the Eulerian and Lagragian solver, is difficult.

- Euler-Euler (EE): Finally, the E-E or continuum approach is at the largest time and length scales where both the gas and liquid phase are solved by phase-averaged equations and the macroscopic effect of interactions between phases is modeled by constitutive equations. Since it is the most computationally efficient this numerical method is particularly suited to model gas-liquid flows in industrial scale equipments. Another advantage of the Euler-Euler model is that
instead of limiting to dilute bubbly flow it can be used to compute any flow regime provided that adequate closure relations about bubble-bubble and bubble-liquid interactions are known. Although more effort is still required to develop phenomenological closure models for bubble forces, turbulence generated by the bubble and bubble dynamics such as bubble coalescence and breakup.

In a general way, two kind of theoretical models for modeling multi phase flow are used. The mixture models, like the Drift flux model [Zuber (1965)] and the models of separated fluids, like the two fluid models [Ishii(1975)] [Ishii and Hibiki(2006)], but both require constitutive relationships to close the model in an analytical way, for some important parameters, like the distribution parameter or the drift velocity in the Drift Flux model, or the friction coefficient and the interfacial area concentration for the two fluids model, require closure relations in order to close the model.

A two phase flow can be described by any of these two models, being the main difference between them the mathematical treatment of the phases, depending the quality of the results on the coupling of the phases, which happens to be the major complication in both cases.

The Drift flux model is used frequently due to is simplicity obtaining the field equations and the constitutive relationships [Cheng(2006)] [Gillard(2007)]).This model is really exact when both phases are strongly connected, and is also recommendable in disperse two phase flow, however, in systems where the inertia of the phases may be considered separately, like the case of annular flow, its application generates numerous doubts. The main hypothesis of this model is that the dynamic of both phases can be expressed in terms of an equation of mixture momentum conservation, being the relative movement between phases specified with a constitutive kinematic equation. The velocity fields are expressed then in terms of the mass center velocity, and the drift velocity of the disperse phase. Given, that the mass and momentum transfer depend on the phase structure, the constitutive relations for the drift velocity and the gas generation are function of the flow regime [Ishii(1975)].

On the other hand, the Two fluids model gives each phase a particular treatment, which consists on establishing for each phase the equations of conservation of mass, momentum, and energy, so that, besides the equations, jump conditions involving the transfer in the interface are needed. This model was formulated by Ishii in 1975 [Ishii(1975)], and in later he would develop a tridimensional model using a temporal averaging (performed at a fixed point over a time interval) and a one-dimensional model using spatial averaging (performed around a fixed point at a certain time).

From these works it was obvious that the interfacial transport terms may be expressed as a function of the product of the interfacial area concentration, and a conductor force of that transference. The interfacial area concentration is a key variable in the closure of
the model, and 2 ways for obtaining it have been proposed, one is the use of empirical correlations, and the other is the use of population balances, that is being developed by some investigation groups [Prasser(2008)], being the interfacial area transport volumetric equation an example of this methodology.

3.2 Two Fluids Model:

Currently the most conventional CFD approach to modeling two-phase flows with significant volume fractions of both phases is the Eulerian two-fluid framework of interpenetrating continua phase distribution, it results from solving the phase-specific continuity equations for volume fractions, and a separate set of momentum equations is solved for each phase. The exchange of momentum between phases is modeled using the correspondent source terms in the phase-specific balance equations. For the dispersed bubbly flows the interfacial momentum transfer is modeled in terms of the drag force due to the hydrodynamic resistance and the non-drag forces. The consideration of the non-drag forces namely the lift, the wall lubrication, the turbulent dispersion force, and the virtual mass force is described in detail.

1. Mass Conservation

The simulations presented in this paper are based on the two-fluid model Eulerian–Eulerian approach. The liquid phase is considered as the continuous phase and the gas phase is considered as dispersed. The flow is isothermal and no interfacial mass transfer takes place. The continuity equation of the two-phases presented by [Ishii (1975)] and [Drew and Lahey(1979)] can be written as:

\[
\frac{\partial \rho_i \alpha_i}{\partial t} + \nabla (\rho_i \alpha_i \vec{u}_i) = S_i \quad \text{Eq.3.1}
\]

2. Momentum Conservation

The momentum equation for the two-phase mixture can be expressed as follows:

\[
\frac{\partial (\rho_i \alpha_i \vec{u}_i)}{\partial t} + \nabla \cdot (\rho_i \alpha_i \vec{u}_i \vec{u}_i) = -\alpha_i \nabla p + \rho_i \alpha_i \vec{g} + \nabla \left[ \mu_i \alpha_i (\nabla \vec{u}_i + (\nabla \vec{u}_i)^T) \right] + F_i + S_{Mi} \quad \text{Eq.3.2}
\]
Where $\alpha_i$, $\rho_i$, $\mu_i$ are the volume fraction, density and viscosity of the phase $i$ and $F_i [N]$ represents the sum of interfacial forces like the drag force, and the considered non-drag forces. The source terms $S_t \left[ \frac{1}{m^3 s} \right]$ and $S_{Mi}$ represent the transfer of gaseous phase mass and momentum between different velocity groups due to bubble break-up and coalescence processes leading to bubbles of certain size belonging to a different velocity group (depending on the case of homogeneous or inhomogeneous MUSIG). Consequently these terms are zero for the liquid phase transport equations. Equations for a mono-disperse bubbly flow appear to be a special case of the previous equations for $N=1$ and $S_t= S_{Mi} = 0$, where $N$ is the number of times the equations have to be solved for the gas phase, that means, the number of considered groups in the gas phase.

3. Energy Equation

\[
\frac{\partial (\rho_i \alpha_i h_{tot,i})}{\partial t} + \nabla \cdot (\rho_i \alpha_i \cdot h_{tot,i} \cdot \vec{v}_i) = -\nabla \cdot \left( \alpha_i (q''_i + q'''_i Re) \right) + p \left[ \frac{\partial \alpha_i}{\partial t} + \nabla \cdot (\alpha_i \vec{v}_i) \right] + \Delta m_i + q_{i,\text{interf}}
\]

\[
\overline{q''_i} = -\lambda_i \nabla T_i; \quad \overline{q''''_i Re} = -\frac{\rho_i n_i}{\rho_i r_i} \nabla h_i
\]

Where, $\lambda_i$ is the thermal conductivity and $\nu_{ti}$ is the turbulent viscosity for phase $i$. $Pr_t$ is the turbulent Prandtl number, $H_{i,\text{interf}}$ is the mean enthalpy of phase $i$ near interfaces, and $\overline{q_{i,\text{interf}}}$ is the interfacial heat flux whose closure won’t be seen in this work as it isn’t necessary. Anyway, since we find ourselves under adiabatic conditions, this equation won’t have to be solved.

3.3 Monodispersed approach.

Monodispersed bubbly flow can be characterized by a single geometrical scale of the dispersed gaseous phase—the bubble diameter, being also called one size approach. Subsequently a two-phase flow model can be formulated describing the liquid and gaseous phase velocity fields and gas void fraction distribution. For a polydisperse bubbly or slug flow with more than a single geometrical scale of the gaseous phase it has been shown by [Tomiyama (1998)], that the lift force acting on bubbles is changing its direction in dependence on bubble size leading to a radial demixing of differently sized bubbles in vertical pipes. This radial demixing of small and large bubbles with respect to the critical bubble diameter in Tomiyama’s lift force coefficient correlation can only be captured by a multiphase flow model, if differently sized bubbles are allowed to move with different velocity fields, therefore, this approach won’t be able to show this effect, by considering a unique bubble size, the lift force will have one
direction or another, either way, no change of sign will be observed., but that will be further reviewed in the MUSIG (Multi Size Group), homogeneous and inhomogeneous.

3.4 Multi-Size Group approach

3.4.1 Homogeneous MUSIG

The two fluid approach assuming a mono-disperse bubble size and applying the described model concepts is not able, to describe the transition from a flow showing a near wall gas volume fraction maximum to a flow with core maximum. For this reason the Eulerian two-fluid approach can be extended to a multi-fluid approach, \textit{i.e.} to simulate a continuous liquid phase and several gaseous dispersed phases solving the complete set of balance equations for each phase. However, investigations showed that for an adequate description of poly-dispersed flows, the inclusion of a population balance model requires decades of bubble size classes. In a CFD code, such a procedure is limited by the increased computational effort needed to obtain converged flow solutions. To solve this problem, the multiple size group model first implemented by the code developers in CFX-4, and solves only one common momentum equation for all bubble size classes (homogeneous MUSIG model, see [Lo(1996)]). Mathematically, the Multiple Size Group model (MUSIG) is based on the population balance method and the two-fluid modeling approach. The dispersed phase is divided into \( M \) size fractions. The population balance equation is used to describe the mass conservation of the size fractions and it accounts for the inter-fraction mass transfer caused by bubble coalescence and breakup. This approach allows a sufficient number of size fraction groups to be used for adequate coalescence and breakup calculations. A number of successful simulations of large-scale industrial multiphase flow problems have shown the applicability of the approach.

Nevertheless, the assumption also restricts its applicability to homogeneous dispersed flows, where the slip velocities of particles are almost independent of particle size and the particle relaxation time is sufficiently small with respect to inertial time scales. Thus, the asymptotic slip velocity must almost instantaneously be attained. Thus, the homogeneous MUSIG model described above fails to predict the correct phase distribution when heterogeneous particle motion becomes important. One example is the bubbly flow in vertical pipes where the non-drag forces play an essential role on the bubble motion. The lift force, as we have already seen numerous times, changes its sign when it is applied for large deformed bubbles, which are dominated by the asymmetrical wake. The radial separation of small and large bubbles cannot be predicted by the homogeneous MUSIG model. This has been shown to be a key mechanism for the establishment of a certain flow regime.
The multi-size approach, is probably the most popular method to calculate bubbly flows with bubble multiple sizes ([Tomiyama and Shimada (1998)]; [Carrica et al. (1999)]; [Lucas, Krepper et al. (2001b)]; [Jones et al.(2003)]; [Chen et al., (2005)]; etc…). This method consists in deciding of a minimal and a maximal values for the bubble diameter \(d_{min}\) and \(d_{max}\) (i.e. an interval \([d_{min}, d_{max}]\) within the different bubble diameters lie) and to split this interval into \(N\) sub-intervals\([d_{i-\frac{1}{2}}, d_{i+\frac{1}{2}}]\) each sub-interval being centered on a discrete value of the bubble diameter \(d_i\). The \(i\)th class, or field, is defined as the set of bubbles having their diameter comprised between \(d_{i-\frac{1}{2}}\) and \(d_{i+\frac{1}{2}}\). See Fig.3. 1 and consider that:

\[
\sum_{i=1}^{N} f_i = 1
\]

The homogeneous MUSIG model solves the transport equations of mass and momentum, for all size fractions \(f_i\):

The source term \(S_i\) from Eq.3. 1 accounts for:

- The birth of bubbles of size \(i\) due to breakup of bubbles of larger size and coalescence of bubbles of smaller size, \(B_{Bi}, B_{Cl} \left[ \frac{1}{m^3 s} \right]\)
- The death of bubbles of size \(i\) due to both break up and coalescence encountered in this size group, \(D_{Bi}, D_{Cl} \left[ \frac{1}{m^3 s} \right]\).

\[
S_i = B_{Bi} - D_{Bi} + B_{Ci} + D_{Cl}
\]
These rate terms may further be expressed as:

\[
B_{Bi} = \rho_i \alpha_i \left( \sum_{k<i} \Omega(m_k, m_i) f_i \right)
\]

Eq.3. 6

\[
D_{Bi} = \rho_i \alpha_i \left( f_i \sum_{k<i} \Omega(m_i, m_k) \right)
\]

Eq.3. 7

\[
B_{Ci} = (\rho_i \alpha_i)^2 \left( \sum_{k<i} \sum_{k<j} \Gamma(m_i, m_k) X_{kji} f_i f_j \frac{m_i + m_k}{m_k m_i} \right)
\]

Eq.3. 8

\[
D_{Ci} = (\rho_i \alpha_i)^2 \sum_{j} \Gamma(m_i, m_k) \cdot \frac{1}{m_k} f_i f_k
\]

Eq.3. 9

Where \( \Omega(m_k, m_i) \) \( \left[ \frac{1}{s} \right] \) and \( \Gamma(m_i, m_k) \) \( \left[ \frac{1}{m^2/s} \right] \) are breakup and coalescence kernel functions, respectively, and will be seen in the chapter corresponding to the tool Ansys CFX and the implemented models on it.

In the case of isothermal flows considered here, the multi-field approach consists in solving 2N mass and momentum balance equations for the N different gas fields corresponding to the N sizes, together with the two mass and momentum balance equations for the liquid phase. As the diameters are known and remain at constant values for all the bubble classes, the resolution of interfacial area balance equations is not necessary. This should be necessary in a (more complicated) variant of the method where the bubble diameters would vary in time and space. Here, the bubble coalescence, bubble break-up and gas compressibility phenomena imply mass (and possibly momentum) exchange terms between the different bubble classes.

3.4.2 Inhomogeneous MUSIG:
A concept that came as an enhancement of the homogeneous MUSIG model previously introduced by [Lo (1996)], is a combination of the consideration of different dispersed phases and the algebraic multiple size group model that was proposed to combine both the adequate number of bubble size classes for the simulation of coalescence and breakup and a limited number of dispersed gaseous phases to limit the computational effort [Krepper, Lucas et al.(2005)]. The Inhomogeneous MUSIG model was developed in cooperation with ANSYS CFX and it has been available for use in CFX since its implementation in the version 10 release of the solver ([Shi et al.(2004)]; [Zwart et al.(2003)]; [Frank et al.(2005)]). In the Inhomogeneous MUSIG model, the gaseous dispersed phase is divided into a number of N velocity groups (or phases), where each velocity group is characterized by its own velocity field. The overall bubble size distribution is further represented by dividing the bubble diameter range within each of the velocity groups \( j \) into a number, \( M_j \) \( (j=1 \ldots N) \), bubble sub-size fractions. The population balance model considers bubble coalescence and bubble breakup, which are applied to the sub-size groups. Hence, the mass exchange between the sub-size groups can exceed the size ranges assigned to the velocity groups, which results in the mass transfer terms between the different dispersed phase equations or velocity groups. The
lower and upper boundaries of the intervals for the bubble size fractions can be controlled by either an equal distribution of bubble diameter, an equal bubble mass or it can be based on user definition of the bubble diameter ranges for each distinct bubble diameter fraction. Exactly as for the homogeneous MUSIG, the subdivision should be based on the physics of bubble motion for bubbles of different size, e.g. dissimilar behavior of distinctly sized bubbles with respect to lift force or turbulent dispersion. According to some authors validation work, the calculations have shown that in most cases \( N = 2 \) or \( 3 \) velocity groups are sufficient in order to capture the main phenomena in bubbly or slug flows [Krepper et al. (2008)], [Krepper et al. (2007)]. See Fig. 3. 2.

The inhomogeneous MUSIG solves the transport equations for mass and momentum, for each velocity group \( j \). That means:

\[
\frac{\partial \rho_g \alpha_j}{\partial t} + \nabla \left( \rho_g \alpha_j \vec{u}_j \right) = S_j \tag{Eq. 3.10}
\]

\[
\frac{\partial \left( \rho_g \alpha_j \vec{u}_j \right)}{\partial t} + \nabla \left( \rho_g \alpha_j \vec{u}_j \vec{u}_j^T \right) = -\alpha_j \nabla p + \rho_g \alpha_j \vec{g} + \nabla \left[ \mu_j \alpha_j \left( \nabla \vec{u}_j + \left( \nabla \vec{u}_j^T \right) \right) \right] + F_j + S_{Mj} \tag{Eq. 3.11}
\]

\( S_{Mj} \) represents the transfer of gaseous phase momentum between different velocity groups due to bubble breakup and coalescence processes that causes bubbles of certain size to switch to a different velocity group (secondary momentum transfer due to mass transfer).

Additionally, for each sub-size fraction, \( i \) \( (i=1, \ldots, M_j) \) in the velocity group \( j \), \( \alpha_i \) the continuity equation has to be solved:
The source terms $S_{ij}$ represent the local transfer of gaseous phase mass due to bubble breakup and coalescence processes, as it has been seen for the two fluid model and the homogeneous MUSIG approach. They can be assigned to $S_i$ for the homogeneous approach of Eq.3.5 which are the elements of the population balance model, having the form:

$$S_i = B_{Bi} - D_{Bi} + B_{Ci} + D_{Ci}$$  \hspace{1cm} \text{Eq.3.13}

### 3.5 Interfacial area transport equation:

The method of interfacial area transport equation (IATE) was first proposed by Ishii and his coworkers [Ishii and Mishima(1981)], [Kocamustafaogullari et al(1995)]. It is based on the intuition that in a two-phase flow the interfacial area density is of importance, since it determines directly the interfacial transfer processes. Therefore, a transport equation is introduced to trace the evolution of interfacial area density. Instead of a globally mono-disperse flow in the standard multi-fluid model a local equivalent bubble size can be obtained from the interfacial area density if the shape of the bubble is specified. The equivalent bubble size is adopted for the calculation of interfacial transfer terms in the extended multi-fluid model. On the other hand, the velocity of the dispersed phase in the multi-fluid model is used as the convective velocity of interfacial area density in the transport equation. No additional mass and momentum conservative equations are introduced. However, it can only model a change of bubble size but not a change of bubble shape since the shape of bubble has to be specified for the calculation of equivalent bubble size. Recently, the concept of two-group IATE has been proposed by Ishii and his co-workers in [Ishii et al (1998)], [Uhle et al.(1998)] and [Wu et al.(1998b)] as a more general model. In this approach bubbles are divided into two groups, i.e. the spherical/distorted bubble group and the cap/slug bubble group. For each group a separate transport equation is solved for interfacial area density. In addition a mass equation and a momentum conservative equation are needed to be solved for each group. For the particular case of two group interfacial area transport equation, it isn’t only necessary to define the breakup and coalescence mechanisms of each group, but also the interactions between these two groups.

Basically, the interfacial transport of mass, momentum and energy are proportional to the interfacial area concentration and to a driving force. This area concentration, defined as the interfacial area per unit volume of the mixture, characterizes the kinematic effects; therefore, it must be related to the structure of the two-phase flow. The driving
forces for the interface transport characterize the local transport mechanism and they must be modeled separately.

Since the interfacial transfer rates can be considered as the product of the interfacial flux and the available interfacial area, the modeling of the interfacial area concentration is essential. In two-phase flow analysis the void fraction and the interfacial area concentration represent the two fundamental first-order geometrical parameters. Therefore, they are closely related to two-phase flow regimes. However, the concept of the two-phase flow regimes is difficult to quantify mathematically at a local point, because it is often defined at the scale close to the system scale. This may indicate that the modeling of the changes of the interfacial area concentration directly by a transport equation, namely interfacial area transport equation is a better approach than the conventional method using the flow regime transitions criteria and regime dependent constitutive relations for interfacial area concentration. This is particularly true for a three-dimensional formulation of two-phase flow.

Different phenomena, that create or absorb interfacial area, such as bubble breakup and coalescence respectively, are taken into account through source terms on the right hand side of the transport equation. Nevertheless, these size-dependent source term processes can hardly be correctly predicted by the assumption of one or two bubble size groups.

Since the interfacial area of the fluid particle is closely related to the particle number, the interfacial area transport equation can be formulated based on the Boltzmann transport equation ([Kocamustafaogullari et al(1995)]; [Ishii and Kim (2004)]):

$$\frac{\partial a_i}{\partial t} + \nabla \cdot (a_i v_i) = \frac{2}{3} \left( \frac{a_i}{a_g} \right) \left( \frac{\partial a_g}{\partial t} + \nabla \cdot (a_g v_g) - \eta_{ph} \right) + \frac{1}{3\psi} \left( \frac{a_g}{a_i} \right)^2 \sum_j R_j + \pi D_{bc}^2 R_{pi} \tag{Eq.3.14}$$

Where the left-hand side represents the time rate of change and convection of the interfacial area concentration. Each term on the right-hand side represents the rates of change of the interfacial area concentration due to the particle volume change caused by the change in pressure, various particle interactions and phase change, respectively. $\psi$ is a shape factor given by: $\psi = \frac{1}{36\pi} \left( \frac{D_{sm}}{D_e} \right)^3$ and is also used to define the particle number density $n = \psi \frac{a^3}{a_g}$, and related to our variables $a_i = nA_i$ ; $a_g = nV$. The Sauter mean diameter is given by: $D_{sm} = 6 \frac{a_g}{a_i} [m]$, and $D_e [m]$ is a volume-equivalent diameter for non-spherical bubbles. $D_{bc}$ is the critical bubble size that should be determined depending on the given nucleation process; namely, the critical cavity size for the bulk boiling or condensation process, and the bubble departure size for the wall nucleation.
As it can be seen, each $R_j$ should be modeled independently, based on the given particle interaction mechanisms. Hence, the mechanistic models of the number source and sink rates for the coalescence and disintegration mechanisms, or those for the bubble nucleation and condensation phenomena, should be established as constitutive relations to solve the transport equation.

Although we won’t start to do so yet, in the following chapter the term $\phi_j$ will be used, referring to $\phi_j = \frac{1}{3\phi} \left( \frac{d}{d_t} \right)^2 R_j$. Except for: $\phi_{ph} = \pi D_{ph}^2 R_{ph}$.

### 3.6 Present Forces and closure relations for the momentum exchange:

An air bubble adopts a shape where surface tension force, hydrostatic forces and hydrodynamic force are in balance at every point of the bubble surface. The hydrodynamic force due to internal gas motion is usually negligible [R. Clift (1978)]. Main forces governing the bubble shape are surface tension, buoyancy, viscous and interfacial forces. The viscous, buoyancy and inertial forces are trying to distort the shape, while the surface tension force is trying to maintain the bubble shape.

At the interface between a gas bubble and surrounding liquid, a balance between the normal force, the viscous force, buoyancy, and the surface tension force must be maintained for gas bubble stability. This balance governs the shape of the fluid particle.

If there is a relative motion of a gas bubble that exists in the surrounding liquid, the shape is naturally influenced by the forces in this surrounding liquid.

#### 3.6.1 Surface tension and viscous force:

If the system pressure and the temperature are constant or their variations are negligible, those forces which change with the bubble diameter and bubble relative velocity are as follows:

- **Surface tension force:** $F_{st} = \pi d_b \sigma$ Eq. 3.15
- **Viscous force:** $F_{vis} = \mu \pi d_b u_b$

Where $d_b$ is air bubble diameter, $u$ air bubble velocity, $\mu_l$ is liquid viscosity and $\sigma$ is air-liquid surface tension. The units have all been already introduced, since all the variables have already appeared. For deformed bubbles, it is customary to define a volume equivalent bubble diameter, $D_{sm}$, corresponding to a spherical bubble of the same
volume of the observed bubble, and, in general, as it has already been seen: \( D_{sm} = 6 \frac{\alpha}{a_t} \)

Where \( \alpha \) is the void fraction and \( a_t \) [\( \frac{1}{m} \)] the interfacial area. Given the case it only has to be substituted in the above-shown equations.

The surface tension force, when it has a constant value over the surface, acts to minimize the surface energy and therefore tends to keep a pure fluid particle spherical in shape [R. Clift (1978)]. Gas bubble will deform only when it is subject to non-uniform or non-symmetric forces such as those due to motion, pressure, or temperature variations that may overcome the stabilizing influence of surface tension.

When the shape of the bubble is deformed considerably, theoretical approaches have limited success to predict the exact bubble shape. The predictions become less accurate with increasing bubble size and deformation because of increasing error in the expected or calculated bubble surface dynamic pressure distribution. Some consequences of this will be commented in the simulations chapter.

### 3.6.2 Modeling of the forces acting on a bubble:

The total force acting on a bubble rising in a liquid can be decomposed into separate and uncoupled contributions of buoyancy, drag, lift, virtual or added mass, wall lubrication effect, and turbulent dispersion (from left to right).

That way the total force acting on a bubble would be given by:

\[
\vec{F}_{tot} = m_b \frac{d\vec{u}_b}{dt} = \vec{F}_B + \vec{F}_D + \vec{F}_L + \vec{F}_{VM} + \vec{F}_{WL} + \vec{F}_{TD} \quad \text{Eq.3.16}
\]

#### 3.6.2.1 Buoyancy force:

The force acting on a bubble due to gravity and pressure gradient, which is also called the buoyancy force, results in a net upward force. The equation for the gravity force is given by:

\[
\vec{F}_G = m_b \ddot{g} = \rho_g V_b \ddot{g} \quad \text{Eq.3.17}
\]

Where \( V_b \) is the bubble volume. The force acting on a bubble due to the pressure gradient in the liquid phase incorporate contributions from the Archimedes displacement force, inertial forces and viscous strain in the liquid:
Getting that way the buoyancy force:

\[ \vec{F}_B = -V_b \Delta P = -\rho_l V_g \vec{g} \]  
\[ \text{Eq. 3.18} \]

\[ \vec{F}_B = \vec{F}_G + \vec{F}_P = (\rho_g - \rho_l) V_b \vec{g} = (\rho_g - \rho_l) \frac{\pi}{6} d_b^3 \vec{g} \]  
\[ \text{Eq. 3.19} \]

### 3.6.2.2 Basset or history force:

When a particle/bubble is subjected to acceleration, because of viscosity, there is a time lag before the surrounding fluid can adapt to the new conditions. The Basset term accounts for viscous effects and addresses this temporal delay in boundary layer development as the relative velocity changes with time. It is also known as the "history" term. The Basset force is difficult to implement and is commonly neglected for practical reasons. It is important when the fluid is almost static and highly viscous. Therefore, not considered in our balance.

### 3.6.2.3 Drag force:

The drag force represents the drag of one phase over the other, and generically, the drag force experienced by the dispersed phase d per unit volume is:

\[ \vec{F}_D = \frac{3}{4} C_D \alpha_d \rho_c \frac{d_b}{u_d - u_c} (u_d - u_c) \]  
\[ \text{Eq. 3.20} \]

Where c, d indicate the continuous and dispersed phase, respectively. It is to clarify, that the subscripts d (dispersed phase) and c (continuous phase) will be used as well as l (liquid) and g (gas) indistinctly, meaning exactly the same.

This equation describes the force’s vectorial form, per unit of volume. It is important to remind the reader that we are always speaking of forces per unit of volume, since the calculation codes, namely CFD, Ansys CFX, don’t work with single bubbles, but with cells with a certain quantity of the disperse phase, being the models the ones that assign to the cells a certain number of bubbles. For as they are n bubbles occupying a volume \( V_b \cdot n \), but for the code it’s only a volume of gas. That way, the force it calculates thanks to the model is multiplied by the volume of gas contained in the cell to obtain the total force to be applied in that cell due to drag. In this case, the same will be done for the other forces. This works in general for all eulerian-eulerian codes. This form of the drag force is the one implemented in our code, differing the models in the expression for calculating the drag coefficient \( C_D \).
Schiller-Naumann model [Schiller and Naumann(1933)]: It’s an adequate model when the particles may be considered as non-deformable solids. This may be supposed it the bubble Reynolds is low, for very viscous fluids, with no distortion of the bubble. That means, although [Schiller and Naumann(1933)] proposed a correlation originally for solid particles, it is also suitable for the case of sufficiently small fluid particles or viscous regime.

\[ C_D = \frac{24}{R_e_p} (1 + 0.15R_e_p^{0.687}) \]  

Eq.3. 21

Where it mustn’t be forgotten that the Reynolds number of the bubble (particle) is given by:

\[ R_e_p = \frac{\rho | \bar{u}_d - \bar{u}_c | d_b}{\mu_l} \]  

Eq.3. 22

On the other hand the models of Ishii-Zuber or Grace consider the bubble distorted, what happens when the Reynolds is high.

Ishii-Zuber model: For the distorted fluid particle regime, the [Ishii and Zuber(1973)] correlation gives:

\[ C_D = \frac{2}{3} E_o^{1/2} \]  

Eq.3. 23

Where \( E_o \) is Eötvös number defined as:

\[ E_o = \frac{g \rho d^2}{\sigma} \]  

Eq.3. 24

Similarly, for dense distributed particles, the previous equation will be modified according to the shape and volume fraction of the particles.
Grace model [Grace (1982)]: It was formulated originally for flow past a single distorted bubble, which is assumed to be applicable for sparsely distributed fluid particles in the distorted regime:

\[ C_D = \frac{4 g d \sqrt{\rho}}{3 u_t^2 \rho_c} \quad \text{Eq.3. 25} \]

Where \( u_t \) is the terminal velocity, given by:

\[ u_t = \frac{\mu_c}{\rho_c d_b} M_o^{-0.149} (J - 0.857) \quad \text{Eq.3. 26} \]

Where \( M_o \) is the Morton number and \( J \) is defined as:

\[ J = \begin{cases} 
0.94 H^{0.751} & \text{if } 2 < H < 59.3 \\
0.32 H^{0.4411} & \text{if } H > 59.3
\end{cases} \quad \text{Eq.3. 27} \]

And \( H \) like:

\[ H = \frac{4}{3} E_o M_o^{-0.149} \left( \frac{\mu_d}{\mu_{ref}} \right)^{-0.14} \quad \text{Eq.3. 28} \]

Where \( \mu_{ref} = 0.0009 \text{ Kg/ms} \) is the viscosity of the reference water.

For the case of densely distributed fluid particles, the previous equation is modified using a power law correction:

\[ C_D = C_{Doo} \alpha^p \quad \text{Eq.3. 29} \]

Where \( C_{Doo} \) is the single bubble drag coefficient and \( p \) is the volume fraction correction exponent depending on the bubble size. This correction exponent is, by default, zero. If there are cases where the group of bubbles can’t be considered as totally diluted, that means, that they don’t influence each other, it is possible to include a correction coefficient to take into account this effect. This way, for small bubbles, this will tend to move slower when doing it together with high void fractions due to the increase of the mixture viscosity, getting the exponent negative values, normally between 0 and -1. For bigger bubbles, they tend to move faster at high void fraction due to the wake entrainment, being the exponent positive.
Tomiyama’s model [Tomiyama(1998)]: Recently, a correlation of drag coefficient was proposed by [Tomiyama(1998)] for pure systems based on single bubbles rising in a stagnant liquid, which is an extension of the model of [Schiller and Naumann (1933)] in the following equation:

\[
C_D = \max \left\{ \min \left( \frac{16}{Re_p} (1 + 0.15Re^{0.687}), \frac{48}{Re_p} \frac{E_o}{E_o+4} \right) \right\}
\]

Eq. 3.30

But apart from this in 2004 Tomiyama proposed a correlation for \(C_D\) for contaminated water (majority of the cases), which requires the following previous definition:

![Elliptical distorted bubble](image)

Mean aspect ratio:

\[
E_{or} = \frac{1}{1+0.163E_o^{0.757}}
\]

Eq. 3.31

Function F:

\[
F(E_{or}) = \frac{1 - \cos E_{or}}{1 + E_{or}} \sqrt{1 - E_{or}^2}
\]

Eq. 3.32

Function G:

\[
G(E_{or}) = \frac{1}{1 + E_{or}^2} \left( \frac{1}{\tanh \left( \frac{E_{or}^2}{E_{or}^2-1} \right)} \right)
\]

Eq. 3.33
Then:

$$C_D = \begin{cases} 
\frac{16}{\text{Re}_p} \left( 1 + 0.015 \text{Re}_p^{0.687} \right) & \text{if } d_b < 0.8 \text{mm} \\
\frac{3}{2} \frac{E_0}{E_0 E_0 + 16 E_{or}^3} \left( \frac{1}{1 - E_{or}} \right)^4 & \text{if } d_b \geq 0.8 \text{mm and } E_{or} > 1 \\
\frac{1}{E_{or} - 1} \left( \frac{4}{E_{or}} \right)^{\frac{4}{3}} \frac{1}{6} & \text{if } E_{or} = 1 \\
\frac{2}{E_{or} E_0} E_0 + 16 E_{or}^3 & \text{if } E_{or} > 1 
\end{cases}$$

Eq. 3.4

The correlation between the mean aspect ratio and the Eötvös number has the form defined by [Wellek et al (1996)]. But actually Tomiyama developed his equation for the parameter $E_n$ instead of $E_{or}$. For an elliptical bubble like the one shown in Fig.3. 3. It is defined: $E_n = b/a$ (supposing $\beta = 1$ in this case).

This is called the aspect ratio and it is an important parameter especially for the definition of the shape and the type of ellipsoidal bubbles (the axial dimension of the particle is $2b$ while the maximum dimension normal to the axis of symmetry is $2a$). A little more about what happens when the elliptical bubble is strongly distorted, will be seen below.

### 3.6.2.4 Lift force:

If the bubbles move in a fluid where a gradient of velocities exists, it moves with a relative velocity that won’t be constant in its surface, creating an asymmetric distribution of the pressure that generates a net force, the lift force, which acts on the bubble in perpendicular to the relative movement direction. This means that the lift force considers the interaction of the bubble with the shear field of the liquid.

Lots of experiments were done to study the lateral migration of the bubbles and identify the main parameters in it. It was observed, as we already know, that the small bubbles migrate towards the wall and the big ones towards the center. The main parameters affecting the lift force [Hibiki(2007)] are the relative velocity between the particle and its surroundings, the velocity gradient of the fluid around the particle, its own rotation, and its surface if it can be considered slip or no-slip, for example due to the presence of surfactants. The general expression of the lift force is given by:

$$\bar{F}_L = -C_L \rho_c \cdot \frac{\pi d_b^3}{6} (\bar{u}_d - \bar{u}_c) \cdot \text{rot} (\bar{u}_c)$$

Eq. 3.5
Where \( \rho_c \) is the liquid density, \( d_b \) the bubble diameter, and \( \bar{u}_d \) and \( \bar{u}_l \) are the bubble (disperse phase) and liquid (continuous phase) velocities, respectively.

This expression was proposed by Drey and Lahey [Drew(1987)] and Auton [Auton(1987)], and used ever since. But it was originally conceived for rigid spheres, and must, therefore, be changed including, besides the parameters affecting the lateral force, the effects of the bubble surface deformation, that affect its wake structure and the flow around the bubble, modifying the lateral force. Moraga [Moraga(1999)] points that the vortex created within the bubble wake have an effect on the lateral force, mainly when the surface becomes asymmetric, what happens when the bubble size increases, and it should be then included in the lift force expression.

In short it can be said that the bubble size and the complex interaction among the created vortex in its wake, as well as the liquid gradient of velocities play a really important role in this lateral migration. [Serizawa(1988)] [Serizawa(1994)] [Tomiyama(2002)]. One of the most characteristic factors appearing in these cases is the change of sign of the lift coefficient. The classical lift force, which has a positive coefficient \( C_L \), acts in the direction of decreasing liquid velocity. In the case of co-current upward pipe flow, this is the direction towards the pipe wall. Numerical [Ervin and Tryggvason(1997)] and experimental [Tomiyama et al.(1995)] investigations have shown results supporting this effect. A separation of bubbles smaller and larger than a critical diameter at which the lift force changes its sign is observed in all upward vertical pipe flows (even for slug and churn turbulent flow), in the case of medium or large void fraction the effect of the lift force combines with dynamic effects, especially by bubble coalescence and breakup.[Lucas et al.(2011)]

![Diagram](image)

Fig.3. 4: Influence of the lift force depending on the bubble size.
This behavior, originally found for single bubbles of air in glycerol was confirmed by a range of experiments also for gas–water polydispersed flows (e.g. Prasser et al., 2007), for steam–water flow and for different other fluid systems of gas–fluids too. For several flow configurations, this bubble size dependency of the lift force direction leads to the separation of small and large bubbles. This effect has been shown to be a key phenomenon for the development of the flow regime.

Moraga [Moraga(1999)] discusses this point in detail and assigns the same causes to the change of sign, but also including that the rotation and the asymmetries within the bubble wake may influence this effect, quoting works like Taneda’s in 1957, that show even how the rotation of rigid spheres may show asymmetries in its wake and change the lateral force’s sign.

That way it could be said that there are two types of lift force, one due to the gradient of velocities within the fluid and the rotation of the bubble, and other due to the deformation/distortion of the bubble and its effect on its wake, diverting its curse. Still today, a huge experimental and theoretical effort on this field is necessary. Below the main lift coefficient models are explained.

**Tomiyama model:** [Tomiyama (1998)] investigated single bubble motion and derived the following correlation for the coefficient of the lift force from these experiments:

\[
C_L = \begin{cases} 
\min [0.2888 \cdot \tanh(0.121 \cdot Re), f(Eo_d)] & Eo_d < 4 \\
-0.27 & 4 < Eo_d < 10 \\
0 & Eo_d > 10 
\end{cases} \tag{3.36}
\]

Where \( f(Eo_d) \), the Eötvös number function is defined as:

\[
f(Eo_d) = 0.00105Eo_d^3 - 0.0159Eo_d^2 - 0.0204Eo_d + 0.474 \tag{3.37}
\]

The coefficient \( C_L \) depends on the modified Eötvös number \( Eo_d \) given by:

\[
Eo_d = \frac{g \cdot (\rho_l - \rho_g) \cdot d_h^2}{\sigma} \tag{3.38}
\]

Where \( d_h \) is the maximum horizontal dimension of the bubble. It is calculated based on an empirical correlation for the aspect ratio developed by [Wellek et al. (1966)] (for for liquid-liquid contaminated systems) with the following equation:
The critical equivalent diameter also decreases with the saturation pressure, as shown by [Lucas and Krepper (2007)]:

\[ d_h = d_b \sqrt[3]{1 + 0.163 \cdot E \sigma^{0.75}} \]  

**Eq. 3.39**

Fig.3. 5: Lift Coefficient dependency with the bubble diameter, and critical bubble diameter dependency with the saturation pressure

**Brief considerations on the calculation of the lift force in simulations, bubble shape, and flow conditions:**

In contrast to the considerations on bubble shape seen earlier in this section, Tomiyama and Celata in [Tomiyama (2001)], defined that, when looking to a distorted oblate spheroidal bubble like the one shown below. Its major axis is \( a \) and the minor axes are \( b \) and \( \beta b \), like before. The parameter \( \beta \), when different to one, enables us to express various bubble shapes such as a dimpled hemispheroidal-cap \((-1 < \beta < 0)\), a hemispheroidal-cap \((\beta = 0)\), a distorted spheroid \((0 < \beta < 1, \beta > 1)\) and a spheroid \((\beta = 1)\). A dimpled hemispherical-cap and a hemispherical-cap can be also expressed by setting \( a = b \).

![Dimensions and coordinates of a distorted oblate spheroidal bubble. [Tomiyama (2002)]](image-url)
Then aspect ratio $E$ is defined by:

$$E = \frac{b + \beta b}{2a} \quad \text{Eq.3. 40}$$

And an aspect ratio $E_f$ for the frontal part of the bubble by:

$$E_f = b/a \quad \text{Eq.3. 41}$$

They both satisfy:

$$E_f = \frac{2}{1 + \beta} E = \gamma E \quad \text{Eq.3. 42}$$

Where $\gamma$ is called the distortion factor.

This would mean, that the correlation of Eq.3. 39 between the aspect ratio and the Eötvös number, which was defined by Wellek et al. for liquid-liquid contaminated systems, may not be exact in some cases, like ours, where actually the flow develops in rather pure conditions. Having $d_h$, the maximum horizontal dimension of the bubble, a slightly different value, and so the Eötvös number function, and, finally, the lift coefficient expression by Tomiyama. To quantify how different these two functions would be, is not an objective of this work and in our opinion further development is necessary on this field. A new correlation between the aspect ratio and the Eötvös number, may be proposed for purer conditions of air-water systems:

![Fig.3. 7: Aspect ratio-Eötvös number possible correlation](image_url)
And an example of the lift coefficient that would be obtained with Tomiyama’s way of proceeding is also shown in his work and can be observed in Fig. 3. 8, where, as said, it must not be considered as a real value, just an approximation:

![Tomiyama Lift Coefficient Graph](image)

Fig. 3. 8: Possible new Tomiyama’s Lift coefficient for air-water pure systems.

Also, to support these considerations, Grace’s diagram is shown, as well as our possible zone of work, considering, as said, that the measured diameter may not be the biggest one. Grace’s diagram contains three main regimes in which the bubbles have different shapes: The spherical, ellipsoidal and spherical-cap regime. The boundaries between the spherical-cap regime and the other two regimes are relatively well defined. The spherical-cap regime consists of three sub-regimes (spherical-cap, skirted and dimpled.) and the ellipsoidal regime consists of two (wobbling and ellipsoidal).
We would find ourselves somewhere between the ellipsoidal and the wobbling regime. Again, we do not intend to quantify or define this with exactitude, but just try to explain that our bubbles are not perfectly spherical, what may imply that the measured diameter may not be the biggest one, since some considerations regarding this matter will be done in Chapter 7.

Magnaudet Model: This model, as developed by [Legendre and Magnaudet (1998)] is applicable mainly to the lift force of small diameter spherical fluid particles, though it could be applied to non-distorted liquid drops and bubbles. In contrast to the lift force model of Saffman-Mei for rigid solid particles, it accounts for the momentum transfer between the flow around the particle and the inner recirculation flow inside the fluid particle as caused by the fluid friction/stresses at the fluid interface. Therefore the predicted lift force coefficients are about a factor of 2-5 smaller than for rigid solid particles.
The range of validity given by [Legendre and Magnaudet (1998)] is as follows:

\[ 0.1 \leq Re_p \leq 500 \quad Sr = 2\beta \leq 1 \quad \text{Eq. 3.43} \]

The lift force coefficient then predicted by:

\[ C_L = \sqrt{(C_{L, lowRe})^2 - (C_{L, highRe})^2} \quad \text{Eq. 3.44} \]

Where:

\[ C_{L, lowRe} = \frac{6}{\pi^2} (Re_p Sr)^{-\frac{1}{2}} J'(\epsilon) \quad \text{Eq. 3.45} \]

\[ C_{L, highRe} = \frac{11 + 16Re_p^{-1}}{21 + 29Re_p^{-1}} \quad \text{Eq. 3.46} \]

\[ \epsilon = \sqrt{\frac{2\beta}{Re_p}} \quad \text{Eq. 3.47} \]

\[ J'(\epsilon) = \frac{J(\infty)}{(1 + 0.2\epsilon^{-2})^{3/2}} \quad \text{Eq. 3.48} \]

\[ J(\infty) = 2.55 \quad \text{Eq. 3.49} \]

### 3.6.2.5 Wall lubrication force:

Near the wall the liquid velocity over the bubble surface changes, what provokes forces on the bubble that push it away from the wall. The resultant force only acts in the wall vicinity, decreasing in an almost exponential way, and disappearing a few millimeters away from the wall, stopping that way its effect. In the last years the study of the bubbles behavior near the wall has been significant, although it is, still a not fully understood matter.

As it has already been seen for the lift force, the interaction between bubbles and liquid flow with developed velocity gradients causes the migration towards the wall. So, as seen, in an upward bubbly flow the bubbles tend to move towards the wall, where the velocity is lower, as long as they don’t exceed a critical diameter, what means, that a certain bubble accumulation will exist near the wall. In this zone the bubbles have two
kind of possible movements, one sliding parallel to the wall, and another of rebound or collision against the wall, also called “bouncing”. Zaruba [Zaruba (2007)] reports this movements, realizing an experimental and theoretical study about the rebound movement of bubbles against the wall. He concluded that an obvious deformation towards ellipsoidal forms existed, and, through the deformation energy, he deduced the deformation force acting on the bubbles as:

$$f_{\text{def}} = \frac{3\sigma}{D_{eq}^2} \left[ \frac{1}{1 - y^6} \left( 3y + \frac{\text{arcsen}(\sqrt{1 - y^6})}{\sqrt{1 - y^6}} \left( \frac{1}{y^2} - 4y^2 \right) - 2y \right) \right]$$

\( y \equiv \frac{2x}{D_{eq}} \)

This deformation force acts as a resort pushing the bubbles away from the wall. When the bubbles collides with the wall, it deforms, continuing its movement even when its surface already impacted, until it reaches a maximal deformation, finally rebounding in the opposite direction, helped by what is called, the wall lubrication force, but, at a certain distant, its velocity becomes again zero and it is pushed again by the lift force, repeating the same process. It could be said that this force appears due to surface tension, to prevent bubbles attaching on the solid wall. Each time, certain energy is lost due to the drag force opposing the bubble movement, reason why this bouncing eventually stops and the bubbles only keep on with their “sliding” movement. Other important conclusion reached by Zaruba [Zaruba(2007)] is that the bouncing amplitude is indirectly proportional to the liquid superficial velocity, existing also, a critical superficial velocity, below which the bubbles keep their bouncing movement for much longer. Finally, the position of the bubbles near the wall is determined by the equilibrium among the lateral forces. It must be said, that, to be accurate, this rebounds don’t take place against the wall, but against a liquid film formed over it in bubbly flow. This film doesn’t possess a constant thickness, fluctuating as it was pointed by Descamps [Descamps(2008)], who concluded, that, independently to the liquid superficial velocity, a free of bubbles film of about 500 \( \mu \text{m} \) will exist. This has certain implications, first that the bubbles will slip on it, what allows us to model the boundary condition at the wall of the disperse phase, as “free slip”, and in second place, that the impact happens in deformable and changing medium, what makes the modeling more complicated.

The implementation of the wall lubrication force is necessary for the adiabatic two-phase flows, as it reproduces the void fraction peak near the wall [Lucas et al. (2004)]. Krepper (in [Krepper et al. (2007)]) reports that its use at high-pressure wall boiling conditions may be questionable, but it is of primary importance when considering isothermal upward bubbly flow at atmospheric pressure and room temperature.
This bubble force was identified to reflect well the experimental results for fully developed upward vertical flow [Lucas and Krepper (2007)], [Krepper et al. (2008)].

**Antal Model:** According to the model of [Antal et al. (1991)], the wall lubrication force on the dispersed phase can be computed as:

\[
\overline{F_{d,WL}} = -\overline{F_{c,WL}} = -C_{WL} \alpha_d \rho_c |\overline{u_d} - \overline{u_c}|^2 \overline{n_w}
\]

Eq. 3. 51

Where

\[
C_{WL} = \max \left\{ 0, \frac{C_{W1}}{d} + \frac{C_{W2}}{y_w} \right\}
\]

Eq. 3. 52

Different combinations of these coefficients were tested in our work, as it will be seen in the simulations section. Really common and spread values are (-0.0064, 0.016) as proposed by [Krepper, Lucas et al.(2005)] and also the pair of value (-0.025, 0.075) proposed by Krepper and Prasser in [Krepper et al.(2007)]. These were chosen in order to obtain these two effects: achieve a higher absolute value of the wall lubrication force and also extend its action not only at the near wall region, although this force will only be active in a thin layer adjacent to the wall and only up to a cut off distance of:

\[
y_w \leq \left( \frac{C_{W1}}{C_{W2}} \right) d
\]

**Tomiyama model:** Furthermore, [Tomiyama et al.(1998b)] proposed a correlation for the calculation of wall lubrication force:

\[
C_{WL} = -C_W(E_o) \frac{d \cdot \rho_c}{2} \left( \frac{1}{y_w^2} - \frac{1}{(D - y_w)^2} \right)
\]

Eq. 3. 53

This means:

\[
\overline{F_{d,WL}} = -C_W(E_o) \frac{d \cdot \rho_c}{2} \left( \frac{1}{y^2} - \frac{1}{(D - y)^2} \right) |\overline{u_{rel}}|^2 \overline{n_w}
\]

Eq. 3. 54
Similarly to the lift force coefficient, \( C_W \) proposed by [Tomiyama et al.(1998b)] depends on the Eötvös number:

\[
C_W(E_o) = \begin{cases} 
\exp(-0.933E_o + 0.179) & 1 \leq E_o \leq 5 \\
0.007E_o + 0.04 & 5 \leq E_o \leq 33
\end{cases} \quad \text{Eq.3. 55}
\]

As pointed out by Tomiyama, the application of this equation is limited to the case with \( \log(Mo) = -2.8 \) (with \( Mo \) the Morton number) and the value of \( C_W \) has to be tuned for other Morton number systems. Here, \( D \) is the pipe diameter. Hence, although the model was found to be superior to Antal's (Frank et al. 2004 [36]) it is restricted to flows in pipe geometries. As is the case for the Tomiyama lift force correlation, the coefficient \( C_W(E_o) \) is dependent on the Eötvös number, and hence on the surface tension between the two phases.

**Frank Model:** Recently, the Tomiyama’s model was modified by [Frank et al. (2004)] to ensure a continuous dependence on the Eötvös number:

\[
C_W(E_o) = \begin{cases} 
0.47 & E_o < 1 \\
\exp(-0.933E_o + 0.179) & 1 \leq E_o \leq 5 \\
0.00599E_o - 0.0187 & 5 \leq E_o \leq 33 \\
0.179 & E_o > 33
\end{cases} \quad \text{Eq.3. 56}
\]

Finally, [Frank et al.(2008)] generalized the Tomiyama’s model to produce the Frank Wall Lubrication Force model, which has no dependence on pipe diameter, and is given by:

\[
C_{WL} = C_W(E_o) \cdot \max \left\{ \frac{0.1}{C_{WD}} \cdot \frac{1 - \frac{yw}{C_{WC} d_p}}{yw \left( \frac{yw}{C_{WC} d_p} \right)^{p-1}} \right\} \quad \text{Eq.3. 57}
\]

Note that \( C_W(E_o) \) preserves the same dependence on Eotvos number as the Tomiyama model. The cut-off coefficient, \( C_{WC} \), determines the distance relative to the particle diameter over which the force is active. \( C_{WC} = 5 \) gives the same range as the Antal model with default constants. The damping coefficient, \( C_{WD} \), determines the relative magnitude of the force. \( C_{WD} = 100 \) gives the same behavior as the Antal model with default constants. However, Frank et al. found that such high damping of the wall lubrication force was not able to sufficiently counterbalance the Tomiyama lift force in the near wall region. The power-law constant, \( p \), makes the force fall off with a variable potential law relationship: \( F_{dWL} \sim 1/y_W^p \).
It is recommended that $\eta$ belongs to the range: 1.5-2. In extensive validation exercises by Frank et al. (2008) the following model constants were determined in order to produce the best possible agreement with experimental data for vertical bubbly flow in pipes: $C_{WC} = 10; C_{WD} = 6.8; \eta = 1.7$. This last values provide the highest $C_{WL}$ value near the wall.

A small comparison among the models is shown in Fig.3. 10:

![Graph showing Evolution of the Wall lubrication coefficient provided by different models.](image)

**Fig.3. 10:** Evolution of the Wall lubrication coefficient provided by different models.

### 3.6.2.6 Turbulent dispersion force:

The turbulent dispersion force is the result of the turbulent fluctuations of liquid velocity, the turbulent eddies and the drag force that appears between phases, causing the transportation of bubbles from regions of high concentration to regions of low concentration of bubbles (or void fraction), and smoothing the radial gas profiles of gas volume fraction, having, therefore, an important influence on the radial gas volume fraction profiles in vertical pipe flows, since, for example, in case the lift force changes its sign, it’s the only one pushing the bubbles from the center to the wall. The same happens in the case of a bigger concentration near the wall. As it is shown in Fig.3. 11.
Lahey [Lahey (1993)] derived an equation for the force, as always, per unit volume:

$$F_{TD}^d = -F_{TD} = -C_{TD} \rho_c k_c \bar{v} \alpha_d$$  \hspace{1cm} \text{Eq. 3.58}

Where $k_c \left[ \frac{m^2}{s^2} \right]$ is the turbulent kinetic energy of the continuous phase (liquid).

López de Bertodano Model: [Lopez de Bertodano (1991)] proposed a model based on this equation and a way of calculating the $C_{TD}$ coefficient taking into account the non-homogeneous turbulent dispersion as follows:

$$C_{TD} = C_{\mu}^{1/4} \cdot \frac{1}{St(1+St)} \Rightarrow St = \frac{\tau_g}{\tau_l} = \Rightarrow \tau_g = \frac{8 \cdot \tau_b}{3 \cdot C_D |u_{rel}|} ; \tau_l = \frac{3 \cdot C_{\mu}^3 k}{\varepsilon}$$  \hspace{1cm} \text{Eq. 3.59}

Where $C_D$ is the drag coefficient, $\varepsilon \left[ \frac{m^2}{s^3} \right]$ the turbulent dissipation rate, $r_b$ the bubble radius, and $C_{\mu}$ a constant that comes from the $k - \varepsilon$ turbulence model and whose normal value is $C_{\mu} = 0.09$, $\tau_g$ is the response time of the bubbles, and $\tau_l$ the eddies scale of the liquid.
Unfortunately, since in Ansys CFX it is implemented in a way that the $C_{TD}$ needs to be defined, and it is not possible to recommend universal values of $C_{TD}$ for this model. Values of 0.1 to 0.5 have been used successfully for bubbly flow with bubble diameters of order a few millimeters. However, values up to 500 have been required for other situations. See [Lopez de Bertodano (1998)] and [Moraga et al.(2003)]. The more universal Favre Averaged Drag model is recommended for all situations where an appropriate value of $C_{TD}$ is unknown.

**Favre averaged drag model: [Burns et al.(2004)]**

Gosman [Gosman et al.(1992)] proposed another expression:

$$F_{d,TD} = -3 \frac{C_D u_{l,l}}{4 d_B Pr_t} \rho_l \alpha_d |\overline{u_{rel}}| (\nabla \alpha)$$

$$Pr_t = \frac{v_{l,l}^{\text{eff}}}{u_k}$$

Where $Pr_t$ is the turbulent Prandtl number, which normally rounds the unity. Basing on this expression, authors like [Carrica et al.(1999)], [Drew(2001)], or [Burns et al.(2004)] proposed a model based on Favre average of the drag.

The FAD model proposed by [Burns et al.(2004)], based on the Favre average of the drag fluctuation term, is:

$$F_{d,TD} = -C_{TD} C_{TC} \frac{u_{l,l}}{Sc_{TC}} \left( \nabla \frac{\alpha_b}{\alpha_a} - \nabla \frac{\alpha_a}{\alpha_a} \right)$$

$$F_{d,TD} = -C_{TD} \frac{3 C_D u_{l,l}}{4 d_B Pr_t} \rho_l \alpha_d |\overline{u_{rel}}| (\nabla \alpha)$$

Where $C_{TD}$ is a user-modifiable multiplier and $Pr_t$ is, as said, the turbulent Prandtl number for continuous phase volume fraction. These correlations show a proportional dependence on the liquid eddy viscosity $u_l$ and Moraga [Moraga2001,2003] shows that this formulation of the turbulent dispersion corresponds to a diffusion term in the equation of mass. $D = \frac{v_{l,l}^{\text{eff}}}{Pr_t}$
3.6.2.7 Virtual mass force:

It’s a force that takes into account, that, although the bubbles have only a small part of the mass they’d have if they were liquid phase, in order to move they need to displace the film of liquid around them, having to realize then, an extra effort, like if they had inertia, weight, the weight of the mass of liquid displaced through their movement. This is the reason why it’s called virtual mass. For quantifying it, it’s tried to consider the work required to move aside the liquid, which happens thanks to the particle energy. If we consider the kinetic energy of the fluid enveloping the particle, considering that at a certain distance the fluid has no movement: \( E_c = \frac{\rho c}{2} \int u^2 \, d\mathcal{V} \). Considering also, that the bubbles moves with a relative velocity \( U \), as shown in Fig.3. 12

![Fig.3. 12: Bubble moving with a relative velocity U](image)

Where, the integral is calculated in all the fluid. If assuming the liquid as incompressible, the velocity can be expressed as a function of the potential \( \vec{u} = \nabla \phi \)

Where this potential of the fluid around a sphere of radius \( a \) in movement is:

\[
\phi = -\frac{Ua^3}{2r^2} \cos\theta
\]

Where \( r \) and \( \theta \) are the cylindrical coordinates, taking the center of the sphere as origin. What leaves:

\[
E_c = \frac{\rho c}{2} \int \nabla \phi \nabla \phi \, d\mathcal{V} = \frac{\rho c}{2} \int \nabla (\phi \cdot \nabla \phi) \cdot d\mathcal{V}
\]

What applying Gauss is:

\[
E_c = \frac{\rho c}{2} \int \phi \cdot \nabla \phi \cdot \hat{n}dA
\]
Integrating in “S”, the bubble surface. Deriving the potential function, we obtain the radial component of the velocity:

\[ u_r = \frac{\partial \phi}{\partial r} = \frac{Ua^3}{r^3}\cos\theta \]  
Eq.3. 66

And the velocity on the bubble surface \((r = a)\):

\[ u_r = U\cos\theta \]  
Eq.3. 67

What means that, operating on the bubble surface, considering that the normal vector to the surface points inside the bubble (as the sphere has to be seen as the surface around the fluid), and substituting in the kinetic energy expression:

\[ E_c = \frac{\rho_c}{2} \int \frac{U^2 a}{2}\cos^2\theta(a^22\pi\rho\theta)d\theta \]  
Eq.3. 68

What, after integrating and operating:

\[ E_c = \frac{U^3a^3\pi\rho_c}{3} = 0.25 M_f U^2 \]  
Eq.3. 69

Where \(M_f\) is the mass of fluid, or virtual mass, that, as it is seen, is half of the mass of fluid occupied by the bubble, what gives sense to the concept of 0.5 as a default virtual mass coefficient.

The kinetic energy variation is the work realized by the virtual mass force, so the virtual mass force will be:

\[ F_{vm} = \frac{a^32\pi\rho_c}{3} \frac{dU}{dt} = 0.5M_f \cdot \frac{dU}{dt} \]  
Eq.3. 70

In a more general way, it can be expressed as:

\[ F_{vm} = \frac{\nu_0\rho_c}{2} \left( \frac{dU_\theta}{dt} - \frac{dU_\lambda}{dt} \right) \]  
Eq.3. 71
Where $V_b$ is the bubble volumen, now, making it per unit volumen:

$$F_{vm} = C_{vm} \alpha \rho_c \left( \frac{DU_g}{Dt} - \frac{DU_i}{Dt} \right)$$

Eq.3. 72

What makes easier its use in the code. Where, $C_{vm}$ is a coefficient that when applied to this kind of flows normally has a value of 0.5. Mouguin y Magnaudet [Mouguin(2002)] pointed out recently that this coefficient may also be applied to spherical bubbles in viscous flow. For spheroid bubbles, Tomiyama [Tomiyama(2004)] proposed a new correlation for the coefficient, considering it as a tensor, changing therefore its value depending on the spheroid form and the direction.

This force only makes sense when bubble acceleration exists, but for the case of fully developed flow in pipes, since the velocities are, more or less constant, it can generally be said that it has small relevance in comparison to the rest of the forces in our set. Results obtained in tests conducted by Frank et al. [Frank et al.(2008)] showed, in effect, that its influence is of minor importance in comparison with the amplitude of the other drag and non-drag forces. Thus, the virtual mass force was not considered in the simulations presented in this paper.

### 3.7 Two phase flow turbulence Modeling.

There most common turbulence models are:

- **Algebraic models**, which are also called zero equation models, because they do not include differential equations. These models solve only algebraic equations for a turbulent viscosity and turbulent Prandtl number, which replace the corresponding laminar values.

- **One-equation models**, which include an additional differential equation for the turbulent kinetic energy.

- **Two-equation models** that include two additional differential equations, the first for the turbulent kinetic energy and the second for a dissipation rate ($k - \varepsilon$) or a frequency ($k - \omega$).

- **Reynolds stress models** include a formula (algebraic or a differential equation) for each component of the Reynolds stress tensor.
The two-equation models are widely used in the industry since they offer a good compromise between complexity, accuracy and robustness. The most popular models are the standard \( k - \varepsilon \) model and various versions of the \( k - \omega \) model. Alternative formulations are now available, see for example the shear stress transport (SST) model. A major weakness of the normal two equation models is that they are insensitive to the curvature of the streamline and the rationalization of the system [Ansys(2009)].

One proposal of two equation models suggests that turbulence consists of small eddies which are continuously forming and dissipating, and in which the Reynolds stresses are assumed to be proportional to mean velocity gradients. This defines an “eddy viscosity model”.

The eddy viscosity hypothesis assumes that the Reynolds stresses can be related to the mean velocity gradients and eddy (turbulent) viscosity by the gradient diffusion hypothesis, in a manner analogous to the relationship between the stress and strain tensors in laminar Newtonian flow. The models used in this work belong to this hypothesis.

3.7.1 Bubbly flow turbulence Modeling:
Turbulence is one of the important mechanisms that lead to bubble coalescence and breakup. However, its modeling is still an open issue in the simulation of gas-liquid flows. In contrast to single-phase flows, the number of terms to be modeled in the governing equations of a two-phase flow is large. This makes the modeling of turbulence in two phase simulations extremely complex. Two-phase turbulence modeling typically involves two-equation models that are formulated on the basis of single phase models. For gas-liquid bubbly flow, it is commonly assumed that the motion of gaseous bubbles follows the fluctuations in the continuous liquid phase. Accordingly, turbulence stresses are modeled only for the liquid phase, whereas a simple zero equation model is used for the gaseous phase. In the present study a Reynolds Averaged Navier Stokes (RANS) turbulence model (that is, based on the Reynolds decomposition principle and separating the average and fluctuating parts of the turbulence variables), based on the SST model is used for the liquid phase, which belongs to the category of eddy viscosity turbulence models and will be explained in detail in Chapter 5. As said in chapter 2, the production and destruction of liquid turbulence caused by the agitation of bubbles, i.e. the so called bubble-induced turbulence (BIT), is considered by additional source terms or by additional viscosity term, both approaches are explained below.
General Approach

There are in general two different approaches to considering bubble-induced turbulence (BIT) discussed in the literature. They are either to add an additional viscosity term or $k$ and $\varepsilon$ source terms.

**Additional viscosity term**

Similarly to the concept of [Sato et al. (1981)] the BIT is described by an additional algebraic viscosity term, which is added to the molecular viscosity of the liquid phase $\mu_l$ in the same way as the shear-induced turbulence viscosity term $\mu \left[ \frac{kg}{Sm} \right]$:

$$\mu_{eff} = \mu_l + \mu_T + \mu_b \quad \text{Eq.3.73}$$

Where $\mu_{eff}$ is the effective viscosity and $\mu_b$ represents the BIT viscosity, which depends on the gaseous phase volume fraction $\alpha_g$, the bubble diameter $d$ and the relative velocity between the phases:

$$\mu_b = C_s \rho_l \alpha_g d |u_{rel}| \quad \text{Eq.3.74}.$$  

$$\mu_T = C_\mu \rho_l \frac{k^2}{\varepsilon} \quad \text{Eq.3.75}.$$  

A value of 0.6 was recommended by [Sato et al. (1981)] for the constant $C_s$, and a value of $C_\mu = 0.09$. This expression is implemented widely in CFD codes such as Ansys CFX. However, as pointed out by [Sato et al. (1981)] it gives too high a value of $\mu_b$ near the wall. In some cases, it has been, therefore, further improved by taking into account the damping effect of the wall surface on BIT turbulence.

$$\mu_b = \left\{ 1 - \exp \left( -\frac{y^+}{A^+} \right) \right\}^2 C_s \rho_l \alpha_g d |u_{rel}| \quad \text{Eq.3.76}.$$  

Where $\left\{ 1 - \exp \left( -\frac{y^+}{A^+} \right) \right\}^2$ is the damping factor. Although in this work, when using the approach with an additional viscosity term, the Sato model implemented in Ansys CFX will be used, and it does not possess the damping factor.
Additional source terms for \(k-\varepsilon\) or \(k-\omega\) model

The most popular approach for the consideration of BIT is to add additional source terms to the transport equations of \(k\) and \(\varepsilon\) / \(\omega\) (the \(k-\varepsilon\) and the \(k-\omega\) turbulence models will be seen in chapter 5) such as \(\varphi_k\frac{m^2}{s^3}\) and \(\varphi_\varepsilon\frac{m^2}{s^4}\) in the following equations:

\[
\frac{\partial}{\partial t}(\alpha_t \rho_t k) + \nabla(\alpha_t \rho_t \bar{u}_i k) = \nabla(\alpha_t(\mu_t + \frac{\mu_t}{\sigma_k})\nabla k) + \alpha_t P_k - \alpha_t \rho_t \varepsilon + \varphi_k \tag{Eq. 3.77}
\]

\[
\frac{\partial}{\partial t}(\alpha_t \rho_t \varepsilon) + \nabla(\alpha_t \rho_t \bar{u}_i \varepsilon) = \nabla\left(\alpha_t(\mu_t + \frac{\mu_t}{\sigma_\varepsilon})\nabla \varepsilon\right) + \alpha_t \cdot \frac{\varepsilon}{k} (C_{\varepsilon 1} P_k - C_{\varepsilon 2} \rho_t \varepsilon + \varphi_\varepsilon) \tag{Eq. 3.78}
\]

Where, \(C_{\varepsilon 1}\), \(C_{\varepsilon 2}\), \(\sigma_k\), \(\sigma_\varepsilon\) are model constants. The shear-induced turbulence production \(P_k\) is given by:

\[
P_k = \mu_t \left| \nabla \bar{u}_t + \nabla \bar{u}_t^T \right|^2 \tag{Eq. 3.79}
\]

There are a number of models proposed for the calculation of BIT source terms \(\varphi_k\) and \(\varphi_\varepsilon\), which are described in the following section.

3.7.2 BIT Additional Source Terms Models

In most models the production of BIT kinetic energy \(\varphi_k\) is calculated as the work of interfacial forces (e.g. drag force, added-mass force), i.e. the interfacial force multiplied with the local slip velocity.

\[
\varphi_k \propto -|M|^2 \cdot |\bar{u}_{rel}| \tag{Eq. 3.80}
\]

It is worth noticing that the drag force is included in all models, since it is the main source of energy input. Non-drag contributions are considered only in a few models, e.g. the added-mass force considered in the work of [Yao and Morel(2004)].

For the modeling of BIT source term in Eq. 3.78, \(\varphi_\varepsilon\), the destruction of BIT is assumed to be proportional to the production divided by a characteristic time scale, \(\tau\):

\[
\varphi_\varepsilon \propto \frac{\varphi_k}{\tau} \tag{Eq. 3.81}
\]

If the \(k-\omega\) model is used instead, the source term for the turbulence eddy frequency \(\omega\) is calculated according to the transformation \(\varepsilon = \beta^* \cdot \omega k\)
\begin{equation}
\varphi_\omega = \frac{1}{\beta^* k} \varphi_\varepsilon - \frac{\omega}{k} \varphi_k
\end{equation}

Eq. 3. 82

Where \( \beta^* = 0.09 \)

The main difference between the existing models for the BIT source terms is the calculation of the time scale \( \tau \).

Several models for BIT production and destruction, \( \varphi_k \) and \( \varphi_\varepsilon \), exist, such as the [Yao and Morel(2004)] model, [Pfleger and Becker(2001)] model, [Politano et al (2003)] model and [Troshko et al.(2001)] model. A benchmark for a number of correlations was done by [Wörner et al.(2004)] using a DNS calculation of eight bubbles rising in a rectangular duct. Correlations like [Kataoka and Sherizawa(1997)], [Pfleger and Becker(2001)], Morel and others were tested. Being the results shown in Fig. 3. 13.

![Fig. 3. 13 DNS calculations of different closure laws for the bubble-induced turbulence [Wörner et al. (2004)]]

The coordinate \( x_3 \) represents the distance from the wall, and logically the coordinate \( y \) represents the turbulence eddy dissipation rate \( \varepsilon \left[ \frac{m^2}{s^3} \right] \). Computational details can be found in [Wörner et al. (2004)]. As it appears in the plot, the correlation of Morel (in red) is the closest one to the exact term profile. For that reason, it will be the one used in this work, and has been chosen to be implemented by us in Ansys CFX. Since it is the one we’ll use, it will be the only one seen in detail.
**Morel model** [Yao and Morel(2004)]:

In [Yao and Morel(2004)] model, in the calculation of BIT only the work input of the interfacial drag force is considered. The additional source term for the $k$ balance equation is expressed as:

$$
\varphi_k = -C_k \overrightarrow{F_{\beta,D}} \left( \overrightarrow{u_g} - \overrightarrow{u_l} \right) = C_k \frac{3}{4} \frac{C_D}{d} \alpha_g |\overrightarrow{u_{rel}}|^3
$$

Eq. 3.83

It can be seen that the BIT kinetic energy is proportional to the gas volume fraction. Accordingly, the source term for energy dissipation balance equation is:

$$
\varphi_\varepsilon = C_\varepsilon \frac{\varphi_k}{\tau}
$$

Eq. 3.84

In the [Yao and Morel(2004)] model, a value of 1.0 is used for both constants $C_\varepsilon$ and $C_k$. The time scale $\tau$ of the pseudo turbulence destruction was calculated based on a dimensional analysis background. The authors assumed that $\tau$ is dependent on the bubble diameter $d$ with the consideration that the wake region behind a bubble is originally of the same size as the bubble. The larger the wake, the longer will be the time required for its energy to cascade to the smallest turbulence eddy scale before it can be dissipated. Therefore, they gave the characteristic time scale as

$$
\tau = \left( \frac{d^2}{\varepsilon} \right)^{1/3}
$$

Eq. 3.85

It must also be reminded, that this model of BIT is not available in Ansys CFX, and must be implemented and set by the user.