University of California, Irvine

Bubble Dynamics in Multiphase Flow in a T-junction at Moderate Reynolds Numbers

THESIS

Submitted in partial satisfaction of the requirements for the degree of

MASTER OF SCIENCE

in Mechanical and Aerospace Engineering

by

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Abstract of the Thesis

Bubble Dynamics in Multiphase Flow in a T-junction at Moderate Reynolds Numbers

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Master of Science In Mechanical and Aerospace Engineering

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Professor Roger H. Rangel, Chair

The deformation and breakup of droplets and bubbles in an immiscible carrier liquid in micro-channels has been extensively investigated in the literature. In this study, we address the case of bubbles in a T-junction at moderate Reynolds numbers, a problem that is relevant for fluidics and emulsion processing applications. The main features include complex oscillating transients, recirculation stabilization, and bubble stabilization against breakup. In particular, very elongated bubble shapes are observed, which would be unstable in the unbounded case and can be explained in terms of wall-induced distortion of the flow field. We show that wall effects can be exploited to obtain nearly mono-disperse emulsions in confined flows. Surface tension also plays an important role on the breakup of the dispersed phase. Different bubble sizes can be obtained depending on the Capillary number as well as the bubble initial size. A mechanism for finding the non-breakup and breakup regions depending on bubble size is determined. This mechanism is determined with different initial flow rates of the carrier flow. The non-breakup regime allows for the bubble to remain attached to the bottom wall of the T-junction. In the breakup regime, the elongation of the bubble results in a significant delay for breakup, allowing for the study of the breakup time and location. Results are presented for different Ca and Re numbers.
Chapter 1

Literature Review

1.1 Flow in Confined Geometries

Fluidics in Confined Geometries deals with the control and manipulation of fluids in channels with typical dimensions from micrometers to meters. Length scales of centimeters are used in this study. One objective behind having small length scales is to increase the surface-area-to-volume ratio. As a consequence, high heat and mass transfer rates can be achieved in these systems, leading to many applications in reactor technology. In these devices, fluids typically flow at low Reynolds numbers, $Re$, defined as the ratio between the inertial forces and the viscous forces ($Re = \frac{\rho H U}{\mu}$, where $\rho$ is the fluid density, $H$ the dimension of the channel, $U$ the representative fluid velocity and $\mu$ the viscosity). Single-phase flow in this regime is mainly laminar which leads to some undesired effects: mixing is mainly due to diffusion, which is a rather slow process.

1.2 Droplets in Confined Geometries

Fluid drops or bubbles suspended in another immiscible fluid undergo deformation and subsequently breakup into smaller droplets or bubbles when the bulk fluid is subjected to strong shearing flows. The mechanism of such droplet deformation has recently emerged as a subject of multidisciplinary research owing to its relevance to various natural systems. The dynamics of drop deformations turned to be a major focus of theoretical and experimental investigations in multiphase fluid mechanics, from the 1930s through the work made by Taylor [1] to the most recent work [2, 3, 4]. More notably, understanding the drop breakup mechanism became a major challenge for scientists and technologists. Despite significant
progress in recent time [5, 6, 7], drop dynamics is still a challenging front of theoretical and experimental work in order to better understand the breakup mechanisms.

The present study aims to characterize the pre- and post-breakup deformation behavior of bubbles in a T-junction channel condition. Using numerical simulations we show that they can undergo breakup and dispersion in different ways depending upon the degree of channel confinement, in addition to the effects of Reynolds and Capillary numbers ($Ca = \frac{\mu U}{\sigma}$, i.e. the ratio between viscous and capillary stresses). The bubbles or droplets in such flow can have a wide range of sizes compared to the channel dimension. Such devices have several applications, such as chemical synthesis and high-throughput screening [8].

1.3 Droplet dynamics in a T-junction

In comparison with continuous single-phase flow fluid mechanics, the physical behavior of droplet fluidics is more complicated due to the presence of the fluid-fluid interface. Interfacial forces, which are proportional to the surface tension coefficient $\sigma$ and the curvature $\kappa$ of the interface, play an important role due to the small scale of the system. Important dimensionless numbers are the Reynolds number $Re$, the capillary number $Ca$ and the Weber number $We=ReCa=\frac{\rho d^2 U}{\sigma}$.

Breakup of droplets can occur in unconfined or confined geometries. In the former, device is large compared to the droplet size. In both cases, droplets experience an external flow that deforms them and finally break them apart. The fundamental difference between them two is that the shape of the unconfined droplet is a function of the strength of the external flow and its properties, while the shape of the confined droplet also strongly depends on the channel geometry. Pioneering work on unconfined breakup was done in the early 1930s by Taylor [1], who showed that a droplet under steady extensional flow is stretched through a series of steady shapes until reaching maximum steady deformation below which the droplet deforms continuously until it breaks. There exists a critical capillary number $Ca$, which corresponds to the critical length of the droplet. This critical capillary number depends only on the viscosity ratio $\lambda = \frac{\hat{\mu}}{\mu}$ of the fluids inside and outside the droplet. Literature on confined breakup starts quite later, in the early 2000s, with the pioneering work by Link [9], who demonstrated that in confined breakup, there is also a critical droplet length, corresponding to a critical capillary number $Ca$. In confined flow, the channel geometry plays an important
role such that the boundary between breaking and non-breaking regimes depends not only on $\lambda$ and $Ca$ but also on the ratio between droplet length and channel width. Link et al. [9] used stability arguments to predict this transition.

**Droplets in a T-junction channel**

The breakup of droplets in confined geometries, such as found in devices with branching networks and in two-fluid flows in porous media, is markedly different from the breakup of droplets in unconfined extensional or straining flows. Relevant questions are the strength of the flow needed to cause breakup and the mechanism by which this occurs.

Literature on unconfined breakup in Stokes flow dates back to pioneering work by Taylor [1], who showed that under steady extensional flow, there exists a critical strain rate $G$ below which a droplet of radius $a$ is extended and assumes a steady elongated shape with a length $l$, and above which the droplet deforms continuously until it breaks. Expressed as a capillary number $Ca=\frac{\mu Ga}{\sigma}$, where $\sigma$ is the interfacial tension between the fluids. In fact, Stone’s stop-flow experiments revealed many of the relevant and interesting flow features of breaking droplets, such as capillary instabilities similar to the pinching of a cylindrical jet, end-pinching, the formation of satellite droplets, etc., that go far beyond the (pseudo-)steady analysis of the maximum strain rate that a droplet can withstand.

**Work on Microfluidics.** The literature has extensively focused on micro T-junctions with equal arms into which a long droplet or bubble is driven and pushed into both arms. Droplets or bubbles in the junction then breakup. Both numerical and experimental data has been collected and studied [1, 5, 8, 10, 11]. The numerical and experimental work done on bubbles and droplets in T-junctions driven by a main flow focus on micro-devices due to its importance to chemical, biological, medical, etc. industries. In this work, a centimeter-scale T-junction will be analyzed. Comparisons with previous results obtained historically for micro T-junctions are made.

Droplets or bubbles in the junction can either breakup or reach a steady shape; this steady shape might be unstable, in which case the droplet eventually escapes into one of the arms. Link et al. (2004) demonstrated that here too, a critical droplet length exists, corresponding to a critical capillary number. In this confined flow, already on dimensional grounds, the
ratio of droplet length to channel width $\epsilon = \frac{l}{w}$ is relevant, and experiments [8] indeed reveal that the boundary between breakup and non-breakup regimes has the form $Ca = f(\epsilon, \lambda)$, being $\epsilon$ the size ratio. More in the spirit of Taylor’s analysis, Leshansky and Pismen [12] predicted the transition by calculating pseudo-steady droplet shapes using a two-dimensional model in which the capillary instability is not operative. However, their model cannot possibly capture the complex three-dimensional shape of long confined droplets, and the mechanisms that govern the dynamics beyond the critical capillary number, i.e. for breaking droplets, have remained unclear.

The management of droplets inside micro-channels in order to control breakup and get the desired drop dimensions after breakup has been widely investigated. Experimental work has been focused on these aspects since the early 1990s [13]. T-junctions are one most common devices for this strategy. Techniques for producing droplets can be either passive or active, the latter meaning that external fields are activated at the time and on-chip location where droplets need to be formed.

In general, the dispersed fluid phase is brought into a micro-channel by a pressure-driven flow, while the flow of the carrier liquid is driven independently. These two phases meet at a junction, where the local flow field, determined by the geometry of the junction and the flow rates of the two fluids, deforms the interface. Eventually droplets pinch off from the dispersed phase finger by a surface instability. The pinch-off of droplets is largely dictated by the competition between viscous shear stresses acting to deform the liquid interface and capillary pressure acting to resist the deformation, which is expressed by $Ca$. This number ranges between $10^{-3}$ and 10 in most micro-fluidic droplet formation devices. Quantitative predictions of the regimes of drop formation, and the drop size still pose a challenge, although significant progress has been made through analytical and numerical studies [2, 3, 4, 7].
Numerical simulations - as the one shown in Figure 1.1 - based on the VOF (Volume of Fluid technique) have also been conducted [2, 7]. The VOF method has been proved successful for this analysis. The droplet size decreases when increasing Ca for all viscosity ratios between the main flow and the dispersed phase [14], agreeing with experimental data [8].

Studies using a geometry as seen in Figure 1.1 [2, 7] have also focused on studying the process of droplet and bubble formation and breakup in micro T-junction channels and it is concluded that at low Ca numbers breakup is not dominated by shear stresses but by surface tension. A simple scaling relation, based on this assertion, predicts the size of droplets and bubbles produced in the T-junctions over a range of rates of flow of the two immiscible fluids, the viscosity of the continuous phase, the interfacial tension, and the geometrical dimensions of the device.
Symmetric T-junction problem  One main investigation [8] has examined the deformation and breakup of bubbles larger than the channel dimensions in a micro T-junction device, which results in a bubble adapting to the shape of the channel.

Recent studies [3, 4, 7, 8] conclude that the deformation of the bubble can occur under different mechanisms depending on the stage it is going through. First there is a quasi-steady deformation of the bubble. In this stage, the bubble can recover its original shape if the flow is suddenly stopped, driven by the external flow. The second stage is a surface-tension-driven three-dimensional rapid pinching that is independent of the externally applied flow. Here, the bubble will always break. Moreover, these studies reveal that the mechanism responsible for this autonomous breakup is similar to the end-pinching mechanism for unconfined droplets reported in the literature [13]: the rapid pinching starts when, in the channel mid-plane, the curvature at the neck becomes larger than the curvature everywhere else. This critical neck thickness depends strongly on the aspect ratio, and, unlike unconfined flows, depends only weakly on the capillary number and the viscosity contrast between the fluids inside and outside the droplet.

1.4 Two-phase flow simulations in a T-junction

Several studies [16, 17, 18] have addressed the behavior of gas-liquid flow devices such as T-junctions. These simulations take the mix of two immiscible fluids. The analysis of gas-liquid flow systems involving T-junctions is very important for applications to phase separation in gas-liquid transport pipelines, but the complexity of the multidimensional phenomenon of dividing two-phase flow in T-junction needs special modeling [16]. It has been found that based on the fundamental mass, momentum and energy balance equations, the mathematical model enables the prediction of phase distribution and pressure drop through the junction taking into account of the two-phase flow pattern and the flow restriction in the tee-branch [17]. The very good agreement of the numerical simulation results with experimental data validates the mathematical modeling and leads to the conclusion that the developed computational code is a very useful tool for the flow characterization of a T-junction separator.
1.5 Droplets in a Sudden Expansion Confined Geometry

Two-phase flow is found in nuclear, chemical or mechanical engineering where gas-liquid reactors, boilers, condensers, evaporators and combustion systems are often used. The presence of geometrical complexities in pipes may affect significantly the behavior of two-phase flow and subsequently the resulting pressure drop. Therefore, it is an important subject of investigation in particular when the application concerns industrial safety valves. The studies of two-phase flow in straight pipes existing in the literature are numerous [19]. However, investigations of two-phase flow in bifurcation, convergence and bends are rather sparse. The aim of studying these geometries is to find how these geometrical complexities influence the two-phase flow pattern and pressure distribution. In particular, the understanding of the flow in such basic geometries can lead to a better design of safety systems.

Some of the authors that have analyzed two-phase flow in expansion geometries are Janssen et al [17]. Correlations for estimating the pressure change in two-phase flow in this type of piping geometry are reported by these authors. These correlations can be extracted from the conservation equations applied downstream of the sudden expansion. The equations used take into account different parameters of the geometry and the flow such as surface area ratio \( \sigma \), mass quality \( x \) and mass velocity \( G \). The lack of studies in progressive enlargements in two-phase flow in the literature makes such an investigation more appealing.

However, literature in the numerical study of droplet behavior in a sudden expansion confined geometry is still lacking. Problems have been solved using experimental techniques but there is not such a large background in analyzing Re and Ca dependencies in the droplet behavior. This chapter aims to show some insights in the numerical results of the problem.

In a sudden expansion, there is a critical Reynolds of the main flow that produces regions of recirculation. Once these regions are produced, the actual change in area of the flow minimizes as a drop moves downstream. Drops may break up if the acceleration in the expansion regions is maximized. Finding mechanisms to break up one drop will allow for the disruption of a stream of drops, but the flow must be pulsating in order to produce expansions without recirculating zones.
1.6 The role of Computational Fluid Dynamics (CFD)

With the development of high performance computing, CFD has played an important role in the design process of flow systems in e.g. aeronautical, automotive, and chemical industries. With CFD, it is easy to vary the characteristics of the systems such as fluid properties, channel geometries and flow conditions, thus allowing broad parametric variations. This is important in the design process as it can provide a cheap and fast way to design and optimize the system. More importantly, CFD can provide detailed temporal and spatial flow information that is crucial to gain insights into the nature and underlying mechanisms of the flows. For droplet fluidics, CFD allows to simultaneously extract both local and global information on three-dimensional shapes of the fluid interface and the flow variation. Moreover, experiments such as stop-flow experiments and perturbation-free experiments, which are useful for the understanding of the flow behavior but difficult to perform physically in confined fluidic systems, can be numerically performed without much effort. Hence, a complete picture of the dynamical behavior of flows in fluidic systems obtained with CFD simulations is very useful in revealing the fundamental understanding of the flows. Various numerical methods has been proposed and used to model flows in droplet fluidic systems, each having its own advantages and disadvantages [20]. Therefore, a careful selection of numerical methods to be applied is crucial. An optimized computational setting can provide a big improvement, sometimes up to a hundred percent, in accuracy and efficiency of the numerical simulations.

SC/Tetra

SC/Tetra, from Cradle [23], is a commercial interactive program used to solve fluidic problems with CFD tools. It is a powerful tool that has the most current improvements in mesh generation and multiphase flow interaction. It is used to solve the mathematical equations which represent the momentum transfer in a moving fluid. These equations are, for constant density, continuity, the three dimensional Navier-Stokes equations in the flowing fluid and the VOF method for the multiphase flow problem:

- Continuity

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0
\]  

(1.1)
• Momentum

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + g_x
\]  \hspace{1cm} (1.2)

\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + g_y
\]  \hspace{1cm} (1.3)

\[
\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} + w \frac{\partial w}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + \nu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) + g_z
\]  \hspace{1cm} (1.4)

• VOF method:

\[
\frac{\partial C_m}{\partial t} + v \cdot \nabla C_m = 0
\]  \hspace{1cm} (1.5)

\[
\sum_{m=1}^{n} C_m = 1
\]  \hspace{1cm} (1.6)
Chapter 2

Objective and Development of Present Study

2.1 Objective of Present Study

This thesis aims to describe the two-phase fluid flow conditions developed in a confined geometry. The confined geometry chosen for this analysis is a T-junction, a device that allows for bubble breakup and deformation.

The objective of this study is the analysis of the bubble dynamics in a carrier liquid inside a centimeter-scale T-junction. The study focuses on moderate Re numbers, ranging from 1 to 50 and Ca numbers ranging from 0.01 to 1. These ranges added to the variation of the viscosity of the bubble (λ ratios) provide a wide picture of bubble dynamics in these conditions.

These dynamics are characterized by different breakup regimes linked to the bubble: from non-breakup to breakup with different bubble satellites. The non-breakup regime is characterized by an attachment of the bubble to the bottom wall of the T-junction. The breakup regime has a clean bubble breakup. The bubble never reaches the bottom of the T-junction, splitting in various pieces. A large piece usually remains, but smaller satellites may appear in these breakups. Changing the size of the bubble changes the size ratio (with respect to the width of the channel): the limits of non-breakup and breakup differ depending on the effect of the surface tension. These limits depend therefore on the size ratio and Ca number, as
proved by [12]. The objective of this study is to find the boundaries between breakup regions.

A transition region between the non-breakup and breakup regimes is also observed. Although the bubble ends up breaking in a large piece, the attachment to the bottom wall of the T-junction is observed. Even though the bubble mostly remains attached to the bottom wall of the T-junction, the inertia of the carrier liquid is enough to eventually cause bubble breakup.

To summarize, the goal of this study is to provide a complete picture of bubble dynamics in a centimeter-scale T-junction device: different Re, Ca and $\lambda$ are studied. Moreover, a pattern for the bubble breakup regime can be found and it is possible to study the volume ratio between the bubble that remains after the breakup and the original bubble.

### 2.2 Development of Present Study

A T-junction geometry is a rectangular duct in which a leading channel splits into two shorter branches. The carrier fluid enters the inlet section located at the beginning of the main channel and bifurcates to the outlet sections in each of the two branches. The square section is 1x1 cm. The main channel length is 4.5 cm and the two branches are 2 cm long as seen in the following pictures.
Figure 2.1: T-junction geometry.
There are two planes of symmetry in this geometry, the Y=0 and the X=0 planes. The carrier liquid enters at a known velocity. The boundary conditions for both outlets is set to a 0 Pa gauge pressure condition. The main fluid flow develops and is allowed to reach a steady condition. Once this is reached, a bubble of a given size, viscosity and a surface tension between both fluids is placed at the inlet, as seen in Figure 2.1.

This bubble is then carried by the main fluid flow. The study focuses on when this bubble eventually reaches the bifurcation. The breakup or non-breakup regimes will occur in this area. Figure 2.3 shows one of the possible scenarios due to the bifurcation (depending on Re, Ca and $\lambda$).
Figure 2.3: 2D view of the T-junction. Bubble elongation due to bifurcation in T-junction
Chapter 3

Numerical Work

3.1 Physical and Numerical Approach for the motion in the T-junction

The problem is treated as incompressible and laminar, viscosity is constant and gravity is neglected. The finite element method is used to discretize the flow domain, thereby transforming the governing PDEs into a set of algebraic equations whose solution represent an approximation to the exact analytic solution.

Election of fluid properties

The properties specified will be:

- Density ratio between both fluids, $\rho = 0.001$. It will be constant throughout the entire study.

- Viscosity ratio between both fluids, $\lambda$. Initially set at $\lambda = \lambda_1 = 0.01$, but it will be changed in the viscosity analysis.

- Surface tension ($\sigma$) between both fluids

- Carrier is liquid.

- Bubble is of a lower density than the carrier liquid.

- Bubble size, which will be constant throughout the entire study.
Analysis conditions

As described earlier, once the carrier flow reaches steady conditions, the bubble is added to the flow.

Solver conditions

The governing equations are the continuity equation, the momentum conservation equation in the three directions and the VOF method when the bubble is added to the main flow.

The numerical method used for coupling velocity and pressure is the PISO algorithm [20], used in addition to an Implicit Euler [21] for the time discretization. Convergence is reached when the difference between two iterations is $1e^{-006}$ or less. To reach this level of convergence, the pressure requires up to 500 iterations whereas the three components of velocity never use more than 10.

The time-step is chosen from the Courant number, which is set to 0.25 [22].

Non-dimensionalization of the problem

The two most important non-dimensional numbers of the problem are:

- Reynolds number, $Re = \frac{\rho I UD_h}{\mu}$, where $\rho_I$ refers to the density of the carrier liquid, $U$ is the inflow normal velocity, $D_h$ is the hydraulic diameter and $\mu_I$ is the viscosity of the carrier liquid. Since the geometry will not change for the entire analysis and according to $D_h = \frac{4P}{A}$, $D_h = 0.01$ m.

- Capillary number, $Ca = \frac{\mu U}{\sigma}$, which represents the relative effect of viscous forces versus surface tension acting across the interface between the liquid and the bubble. $\sigma$ refers to the surface tension across the interface.

Some other non-dimensional numbers that affect the solution are:

- Viscosity ratio, $\lambda = \frac{\mu_B}{\mu_I}$, it is the ratio between the viscosity of the bubble to the viscosity of the liquid.

- Bubble size ratio, $\epsilon = \frac{d}{w}$, where $d$ is the diameter of the bubble and $w$ is the width of the channel.
• Non-dimensional time, \( \tau = \frac{u t}{w} \), which is used to compare bubble dynamics in the bifurcation. \( U \) is the inflow normal velocity and \( w \) is the width of the channel.

• Non-dimensional breakup distance, \( \delta = \frac{x}{L} \), where:

![Figure 3.1: Breakup Distances for Analysis I](image)

• Non-dimensional bubble neck (always referred to the thinnest part of the elongation of the bubble) thickness, \( \eta = \frac{z}{w} \), where:

![Figure 3.2: Breakup Distances for Analysis II](image)

• Non-dimensional neck elongation, \( \delta_c = \frac{z}{L} \). That occurs when the bubble neck is displaced from the center of the T-junction due to the bubble elongation. It is:
Numerical mesh

A balance between accuracy in results and computation time is used to choose the number, size and distribution of finite elements throughout the solution domain. A hexagonal mesh is used, and the number of elements used vary from 1,200,000 to 5,000,000 in order to show that the results are mesh independent. Consequently, the computing time for each calculation may vary from 9 to 15 hours on an i7 8-core processor until convergence is reached. An hexagonal type of mesh is chosen and, as in any finite element analysis, more elements are required in areas of the model where spatial gradients of the solution variables are high. In this study, locations where the mesh definition requires special attention are the solid boundaries. An example of a mesh is shown in Figure 3.4. Since the length scale of the problem is \( \sim 1 \) cm, a 3 layer refinement at the walls is enough to capture the no-slip condition and the boundary between the matrix fluid and the bubble surface.
3.2 Use of symmetry for numerical convenience and numerical validation

If we wanted to simulate all the cases using the original geometry shown in 2.1 with a proper mesh leading to accurate results the time computation would be too long. One way to reduce the number of elements to use for the FEM but still getting accurate and reliable results is to use the symmetry that the problem itself has. As stated before, there are two planes of symmetry in this problem: X=0 and Y=0.

Applying both symmetries leads to solve the problem with a quarter of the original geometry. We compare the results for the original T-Junction (T-J) with the results for the quarter of the T-junction (quarter of T-J). This also allows to show mesh size independence of the problem, since both cases will use a different hexagonal mesh.

![Figure 3.5: Geometry used for numerical convenience](image)
Problem comparison. Mesh size independence

To prove that one quarter of T-J works well, we compare the solution with two different geometries and, therefore, meshes.

Table 3.1: Number of elements according to the geometry

<table>
<thead>
<tr>
<th></th>
<th>number of elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>T-Junction</td>
<td>4.491.310</td>
</tr>
<tr>
<td>quarter of a T-Junction</td>
<td>2.209.794</td>
</tr>
</tbody>
</table>

Table 3.1 shows that the geometry is one fourth of the original one, but the number of elements is half. This means the mesh is expected to be more accurate in the one fourth of T-junction even though we have a fewer number of elements compared to those of the original geometry.

The following figures show three different simulation times of a typical bubble breakup problem, solved for both cases. The result shown corresponds to the 2D VOF=0.5 of the bubble for the middle plane (Y=0). The problem conditions used in both cases are: $Re = 50$, $Ca = 0.5$, $\lambda = 1$, $\epsilon=0.6$. The boundary and initial conditions are also repeated in both problems. The first simulation time takes into account the bubble before being affected by the channel split. The second simulation time shows the elongation of the bubble due to the bifurcation before breakup, and the third one shows the large satellite remaining after breakup.

The three figures show some lengths used to compare the results with different meshes. All lengths are given in cm.

For the first simulation time, we obtain:
Figure 3.6: Simulation time = 0.028 s. a) shows the 2D result in the reduced geometry, b) shows the 2D result in the whole geometry and c) is the superposition of both results.

The second simulation time, $t=0.05$ s, leads to:
Figure 3.7: Simulation time = 0.05 s. a) shows the 2D result in the reduced geometry, b) shows the 2D result in the whole geometry and c) is the superposition of both.

The third simulation time, t=0.064 s, shows:

Figure 3.8: Simulation time = 0.064 s. a) shows the 2D result in the reduced geometry, b) shows the 2D result in the whole geometry and c) is the superposition of both.
It is required to calculate the distances obtained for L1, L2 and L3 for both meshes, and a comparison between them is made as follows:

Table 3.2: Effect of mesh size

<table>
<thead>
<tr>
<th></th>
<th>T-junction</th>
<th>quarter TJ</th>
<th>% difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>L1 (cm)</td>
<td>1.025</td>
<td>1.028</td>
<td>0.29%</td>
</tr>
<tr>
<td>L2 (cm)</td>
<td>1.119</td>
<td>1.114</td>
<td>0.8%</td>
</tr>
<tr>
<td>L3 (cm)</td>
<td>0.62425</td>
<td>0.61875</td>
<td>0.88%</td>
</tr>
</tbody>
</table>

According to table 3.2, distance L1 refers to the elongation of the bubble in Figure 3.7, L2 refers to the breakup distance in Figure 3.8 and L3 refers to the bubble distance from the bottom of the T-junction as seen in Figure 3.6. The comparisons show a difference smaller than 1%.
Chapter 4

The Steady Problem

As explained so far, the bubble dynamics take place inside the T-junction once the primary fluid flow (the carrier liquid) reaches steady conditions. Therefore, a first simulation in order to reach those conditions is conducted. Taking into account the boundary conditions described before, the only variable changed here is the inflow velocity. This inflow velocity affects the Reynolds number since the liquid density and viscosity and the T-junction dimensions remain constant.

The only remarkable non-dimensional number in this study is the Reynolds number. It affects the state of the carrier liquid once it reaches steady conditions, and therefore, the initial conditions the bubble will encounter once it is added to the main flow. Re-circulation areas start to appear at Re~30. The sudden change in geometry in the T-junction generates a flow motion around the T-junction corners which generate re-circulation regions.

The numerical method uses pseudotimesteps in order to reach the steady condition. The value for the liquid dynamic viscosity, $\mu_l$, is 0.1 Pa·s, the liquid density is $990 \frac{kg}{m^3}$ and the sides of the squared section are 1 cm each.

$Re=1$ The inflow velocity is $U = 0.01$ m/s. The main characteristics of the steady state reached by this inflow in the T-junction are shown in Figure 4.1. The plane showed is the middle plane of the device (Y=0).
The streamlines of this characteristic flow motion show that at this velocity the sudden change in geometry does not disturb at all the fluid flow. Its motion is smooth.

\textbf{Re=10}  The inflow velocity is $U = 0.1 \text{ m/s}$. The main characteristics of the steady state reached by this inflow in the T-junction are shown in Figure 4.2. The plane showed is the middle plane ($Y=0$) of the device.
The inflow velocity is \( U = 0.2 \) m/s. The main characteristics of the steady state reached by this inflow in the T-junction are shown in Figure 4.3. The plane showed is the middle plane (\( Y=0 \)) of the device.
Re=30 The inflow velocity is $U = 0.3 \text{ m/s}$. The main characteristics of the steady state reached by this inflow in the T-junction are shown in Figure 4.4. The plane showed is the middle plane ($Y=0$) of the device.

Figure 4.4: Velocity distribution, pressure distribution and streamlines at steady state for Re=30

Re=40 The inflow velocity is $U = 0.4 \text{ m/s}$. The main characteristics of the steady state reached by this inflow in the T-junction are shown in Figure 4.5. The plane showed is the middle plane ($Y=0$) of the device.
**Re=50**  The inflow velocity is $U = 0.5 \text{ m/s}$. The main characteristics of the steady state reached by this inflow in the T-junction are shown in Figure 4.6. The plane showed is the middle plane ($Y=0$) of the device.

Starting at $Re=30$, the streamlines show the formation of a re-circulation zone, due to
the increase in the inflow velocity. Figure 4.7 shows a detail of the re-circulation zone.

Figure 4.7: Streamlines near the wall and the corner of the bifurcation
Chapter 5

Results

The transient problem is solved here. In the previous section, the different steady states of the carrier liquid motion have been shown. The bubble is introduced in these conditions. The consequent deformation, elongation and potential breakup are studied in this chapter. For the study of the Reynolds number effect, the same bubble (same properties) is added to the previous flow configurations.

5.1 Effect of the Reynolds number on the bubble breakup and deformation

When the Reynolds number is larger than 30, re-circulation zones are created. Since the bubble diameter is smaller than the channel width unlike in [1, 2, 8], the re-circulation alters the bubble dynamics. Non-breakup and breakup regimes are expected and a critical Reynolds number for this limit is found. The breakup regime, however, can be divided in three categories. The size ratio is $\epsilon = 0.6$ and viscosity and density ratios will be unaltered ($\lambda = 0.01$, $\rho = 0.001$). Capillary number effects will be considered.

The Reynolds number will vary from 0.005 to 80. Increasing the Reynolds number increases the inertial forces of the carrier flow on the bubble. Therefore, a balance between the surface tension and inertial forces leads us to the different breakup regimes and their limits. Hoang and Fu [8] already demonstrated that this limit can be found changing the size ratio of the bubble.
Three different bubble breakup regimes are observed:

- Non-breakup regime.
- First breakup regime.
- Second breakup regime.

5.1.1 Bubble evolution for different Reynolds numbers

Figure 5.1 shows the evolution of the position of the bubble in the T-junction for different Reynolds numbers (keeping Ca constant), and it illustrates the three different breakup regimes.
Figure 5.1: Evolution of the bubble for different Re and Ca=0.3.

For low Reynolds numbers (Re<0.01), the bubble remains attached to the bottom wall of the T-junction and the bifurcation does not affect its deformation. Previous studies [3, 4] already found a limit in the non-breakup/breakup region: the surface tension effect is stronger than the shear stresses and keeps the bubble together. Since this limit depends on the bubble size as well, it is necessary to increase the Reynolds number if we keep the bubble properties constant. Figure 5.1-(b) shows the breakup behavior of the bubble for Re=1. The evolution of the bubble in these conditions shows a clean breakup into a large piece and a small satellite remaining due to the previous elongation of the bubble. Increasing the inflow velocity, and therefore increasing the Reynolds number increases the contribution of the inertial forces on the bubble deformation. The set of figures 5.1 also shows, when Re=30, a clean breakup taking place outside of the geometry limits of the T-junction device. However, one can still estimate the location and time of the breakup. If the Reynolds number is increased further, no breakup takes place inside the T-junction. However, for Re=50, the effect of the Reynolds number changes. The balance between inertial and capillary forces is different and results in a different breakup regime of the bubble. The Re=50 case is shown in Figure 5.1-(f). There is a qualitative difference in the dynamics of the bubble breakup at
these conditions with respect to lower Re numbers. Figure 5.2 shows a different view inside the T-junction in order to understand this regime.

Figure 5.2: Second breakup regime in the T-Junction

The effect is better observed in Figure 5.3, where the same problem is solved using the
entire geometry of the T-junction.

![Diagram](image)

Figure 5.3: Second breakup regime.

The threshold Re number where this effect starts to take place (for Ca=0.3) is Re=42. The deformation of the bubble is characterized for each Reynolds number. The neck of the
bubble undergoes two different effects: stretching and elongation.

5.1.2 Bubble Stretching

The stretching of the neck is the effect of deformation of the bubble in the direction of the main channel flow. As time progresses, the neck thickness decreases. The time in the analysis is measured from the instant when the entire bubble is inside the bifurcation.

There is an evolution of the neck thickness $\eta$ with time until the bubble breakup. Figure 5.4 shows, for $Re=0.1$, three different times during the motion of the bubble in the T-junction after it has reached the base of the T.

![Figure 5.4: Evolution of the neck thickness of the bubble for Re=0.1 and Ca=0.3.](image)

Figure 5.4 shows that the neck of the bubble stretches as the bubble deforms inside the device. This evolution is completed when the breakup (or non-breakup) is produced. Figure 5.5 shows the evolution of the non-dimensional neck thickness $\eta$ versus non-dimensional time for $Re=0.1$. 
Figure 5.5: Non-dimensional neck thickness versus non-dimensional time for Re=0.1

When $\eta = 0$, the breakup has occurred. What is the deformation of the neck for different Reynolds number at the same non-dimensional time? The answer to this question helps understand the effect of the Reynolds number on the stretching of the neck. Figure 5.6 shows the width of the neck at the same non-dimensional time for different Re numbers.

Figure 5.6: Bubble deformation. Neck thickness for different Reynolds numbers at the same non-dimensional time $\tau$. 
The evolution of the neck thickness is plotted in Figure 5.7 for different Re numbers.

Figure 5.7 shows how in the $0.1 < \text{Re} < 40$ range a common behavior in the evolution of the neck thickness exists. The larger the Reynolds number the faster it stretches but the longer it takes to finally break. For Re=50, the behavior is no longer the same. Now, the bubble is in the next breakup region where the bubble creates a crown before breaking. The stretching is now faster, as well as the breakup. Certainly, the neck thickness evolution can also be explained in terms of the non-breakup. In the non-breakup the bubble remains attached to the bottom wall of the device. The non-breakup regime can be seen in Figure 5.8 for Re=0.0005.
Figure 5.8: Bubble deformation. Non-dimensional neck thickness $\eta$ versus non-dimensional time $\tau$ for different Re numbers, including non-breakup, at Ca=0.3

5.1.3 Bubble Elongation

The elongation of the neck of the bubble is the deformation of the bubble in the direction of the flow. The breakup and evolution of the bubbles in the T-junction can also be studied in terms of the elongation of the bubble neck, as seen in the previous figures. Not only the stretching until breakup but the bubble elongation until breakup ($\delta_c$) is also important in order to characterize the breakup distance and time. Figure 5.4 also shows the elongation for three different non-dimensional times and Re=0.1, Ca=0.3

Figure 5.9 shows the elongation evolution with time for Re=0.1 and Ca=0.3.
Figure 5.9: Non-dimensional neck elongation $\eta$ versus non-dimensional time $\tau$ for Re=0.1 and Ca=0.3

The curve ends when the breakup occurs and the neck elongation is no longer relevant. It is therefore important to study the evolution of this elongation with time for each Reynolds number. Different Reynolds numbers will lead to different elongation distances and times. For instance, Figure 5.10 shows the same non-dimensional time for different Reynolds numbers.
Figure 5.10: Bubble neck elongation for different Re at the same non-dimensional time $\tau$

There is clearly a dependency between the elongation evolution and the Reynolds number of the main fluid flow. Since the non-breakup regime does not satisfy elongation, it will not be shown here. Figure 5.11 shows the non-dimensional neck elongation of the bubble ($\delta_c$) before and until break-up as a function of the non-dimensional time $\tau$.

Figure 5.11: Non-dimensional neck elongation $\delta$ versus non-dimensional time $\tau$ for different Re numbers and Ca=0.3. Inserts show bubble elongation just before breakup for each Reynolds number.
The larger the Re number the longer is the elongation and the final breakup distance. However, this pattern is no longer valid when Re > 42, since the clean breakup region is not present anymore, and shorter elongation and breakup distances are found.

5.1.4 Bubble Breakup

The bubble breakup is the final stage in the deformation of the bubble. After deforming for a while, the neck of the bubble becomes so thin that a breakup occurs, leaving a residual bubble. A satellite leaves the device with the outflow through the outlet. The Reynolds number has an effect on the breakup time and distance. Figure 5.12 shows the two breakups regimes one can expect in these conditions.
Figure 5.12: Breakup patterns

Figure 5.12-(a) shows the clean breakup described earlier. The bubble remains in the symmetry plane $Y=0$ whereas in figure 5.12-(b) there is separation of the bubble from the symmetry plane $Y=0$.

The study of the breakup for different Re numbers include the location and time where and when it occurs. Figure 5.13 shows the non-dimensional breakup time and the non-dimensional breakup distance versus the Reynolds number for $Ca=0.3$. 
(a) Non-dimensional breakup time $\tau$ versus Re number for $Ca=0.3$

(b) Non-dimensional breakup position $\delta$ versus Re number for $Ca=0.3$

Figure 5.13: Non-dimensional breakup position and time versus Re number
Figures 5.13 (a) and (b) show the evolution of the breakup versus the Reynolds number. The effects of the range of Reynolds numbers is noted. Low Re numbers (Re<0.005) do not cause breakup and this effect is shown in (a) since initially the non-dimensional time is infinite. The first noticeable breakup occurs in the range 0.005 < Re < 0.01. Beyond this, there is a constant increase of the breakup time and the behavior is qualitatively similar in the range 0.01 < Re < 40. However, when Re~40, there is a sudden drop in both - position and time - non-dimensional quantities. A different breakup regime is reached. Figure 5.14 offers a better explanation, showing three different breakup positions for three different Re numbers. Inserts (i) and (ii) show the first breakup regime but insert (iii) shows how the bubble encounters the second breakup regime.

Figure 5.14: Non-dimensional breakup position $\delta$ versus Re number for Ca=0.3. Change of breakup pattern.
5.2 Effect of the Surface Tension on the Bubble Breakup and Deformation

The balance between the inertial forces (reflected in the Re number) and the capillary forces leads to the three different regimes that have been described before. Here, Re, λ and ρ are kept constant and we study the effect of the surface tension σ. The boundaries between non-breakup and breakup regimes can also be found for Ca [3] [12] and are determined here. In later sections, the regimes can finally be determined and also their boundaries with respect Re and Ca.

5.2.1 Bubble evolution for different Ca numbers

The following figures show the evolution of the bubble for different Ca numbers keeping the Reynolds number constant. The figures include two different Reynolds numbers in order to see the effects of the change in Capillary forces. Figure 5.15 shows the bubble evolution for different Ca numbers and Re=50, and Figure 5.16 shows the bubble evolution for different Ca numbers and Re=10.

(a) Bubble evolution for Ca=0.05 and Re=50  (b) Bubble evolution for Ca=0.1 and Re=50  (c) Bubble evolution for Ca=0.2 and Re=50
Figure 5.15: Bubble evolution for different Ca numbers and Re=50.
Figure 5.16: Bubble evolution for different Ca numbers and Re=10.

Figure 5.15 shows the three breakup regimes that have been described before. Non-breakup occurs for low values of Ca, as shown numerically [12] and experimentally [9]. It is necessary to lower the value of the surface tension in order to reach clean breakup conditions of the bubble. Figure 5.15-(b) shows the clean breakup once the Capillary number reaches 0.1. Increasing it even more leads to the crown-shaped breakup regime which can be seen in figures 5.15-(d) and 5.15-(e). However, Figure 5.16 shows the same Capillary numbers for a different Re number (Re=10). This figure shows how the bubble does not reach the second breakup regime. This leads to a very important conclusion: since it has been shown that the various regimes so far depend on the balance between inertial forces and capillary forces, it is important to find the boundaries of the breakup regimes for the different combinations Re-Ca.

The study of the bubble breakup in the T-junction device in these conditions will then take into account the stretching of the bubble neck and its elongation until potential breakup.
5.2.2 Bubble Stretching

The deformation of the bubble under these conditions occurs in the direction of the flow in the main channel of the device. In the non-breakup regime, the deformation once it has reached the bottom wall of the T-Junction is very small and the bubble remains attached to the wall for a long time. It is not until the clean breakup occurs that the deformation is important to be studied. Figure 5.19 shows the deformation of the bubble in the same non-dimensional time for different Ca numbers.

![Figure 5.17: Neck thickness for \( \tau = 2.3 \) for different Ca and Re=10](image)

As expected, there is a clear dependency on the evolution of the neck thickness of the bubble \( \eta \) with respect the Capillary number. Figure 5.18 shows the evolution of the neck thickness \( \eta \) versus the non-dimensional time for different Ca numbers and Re=10.
Figure 5.18: Neck thickness $\eta$ versus non-dimensional time $\tau$ for different Ca and Re=10

5.2.3 Bubble Elongation

The elongation of the bubble also depends strongly on the value of the surface tension. Different capillary numbers will lead to different elongation, breakup locations and breakup times. Figure 5.19 shows the elongation at $\tau = 3.7$ for different values of the Capillary number.

Figure 5.19: Bubble elongation for $\tau = 3.7$ for different Ca and Re=10
5.2.4 Bubble Breakup

This section only considers the first and second breakup regimes. In the clean breakup regime, a continuous elongation of the bubble occurs until the neck thickness is so thin that the breakup occurs. The breakup produces a large secondary bubble and leaves behind a piece of the original bubble. This remaining piece is different in the crown-shaped breakup regime. This regime begins at larger values of Ca, or, in other words, lower values of the surface tension if Re is kept constant. Figures 5.20 and 5.21 show the breakup instant for Ca=0.2, 0.3 and 0.4 for two different Reynolds numbers.
Figure 5.20: Breakups for Re=10

(c) Breakup for Ca=0.4
Figure 5.21: Breakup for Re=40

Figure 5.21-(c) shows how the bubble encounters the second breakup regime when increasing Ca. For Re=10, on the contrary, this effect does not take place. Again, these figures show how the combination Re-Ca sets the limits for the breakup regimes. There are other Reynolds numbers where the second breakup regime does not occur even for a large value of Ca. The Ca effect on the breakup pattern has to consider both situations, where the bubble encounters the second breakup regime and where it does not. Figure 5.22 shows
the breakup position $\delta$ and time $\tau_b$ versus Ca number of the flow.

Figure 5.22: Breakup position and time pattern versus Ca number

Figure 5.22 shows the trends in the breakup behavior of the bubble under different...
conditions. For Re=10 and Re=20, the change in the Ca number does not result in the second breakup regime and the linear trend is found either for the breakup position and the breakup time. However, for Re=40 and Re=50 it is possible to see how the Ca number affects the breakup position and time. There is a sudden drop in both. The reason is that for these Reynolds numbers, there is a Ca number limit for which the breakup regime changes. Both the breakup distance and time show this limit.

5.3 Effect of the Viscosity Ratio on the Bubble Breakup and Deformation

So far, the viscosity ratio between the bubble viscosity and the carrier flow viscosity has been kept constant at $\lambda = \lambda_1 = 0.01$. The change in its value leads to different breakup patterns. In fact, the breakup regime boundaries differ depending on the viscosity ratio. An illustration of this is shown in figures 5.23 and 5.24 where the evolution of the bubble is shown for different viscosity ratios.

Figure 5.23 shows the bubble evolution for Re=10, Ca=0.2 and $\lambda = \lambda_1$, $\lambda = 2\lambda_1$ and $\lambda = 0.5\lambda_1$.

Figure 5.23: Bubble evolution for different viscosity ratios $\lambda$, Re=10 and Ca=0.2
Figure 5.23 shows how the change in the viscosity ratio produces a different bubble deformation, since the non-dimensional times shown are the same for the three figures. Increasing $\lambda$ causes a delay in the breakup. A clearer change of pattern is observed in Figure 5.24 for Re=40 and Ca=0.4. With $\lambda = \lambda_1$ the bubble is in the second breakup regime. The following figures show how changing the viscosity ratio can produce a completely different breakup.

![Bubble evolution for different viscosity ratios](image)

Figure 5.24: Bubble evolution for different viscosity ratios $\lambda$, Re=40 and Ca=0.4

It is important to note how $\lambda = 4\lambda_1$ prevents the bubble from reaching the second breakup regime that occurs for $\lambda = \lambda_1$. Figures 5.23 and 5.24 show how sensitive the elongation of the bubble is in front of the viscosity ratio. The following figures go deeper into this concept, and show a clear difference in the bubble elongation (and therefore breakup) for different viscosity ratios. Figure 5.25 shows more clearly the effect of increasing the viscosity ratio. For Re=10 and Ca=0.2, the following pre-breakup situation develops for different viscosity ratios at the same non-dimensional time:
The higher the viscosity ratio the longer the bubble becomes, so the opposite effect is expected if there is a decrease in the viscosity ratio value. Figure 5.26 shows bubble elongations at the same non-dimensional time for different viscosity ratios - lower than the base case:

Figure 5.26 shows the trend: the lower the viscosity ratio, the harder it is for the bubble to deform. Therefore, lowering even more the value of the viscosity ratio must lead to the non-breakup regime. Figure 5.28 shows the change in breakup regime due to the change in the viscosity ratio:
Certainly a change in the viscosity ratio can lead the bubble to a different breakup regime, again. Figures 5.23 and 5.24 showed how a change in the viscosity ratio takes the bubble from the second breakup regime to the first breakup regime. A change in viscosity ratio takes the bubble from breakup to non-breakup. Figure 5.28 shows the elongation of the bubble versus non-dimensional time for different viscosity ratios. Inserts show the eventual breakup instant for each viscosity ratio.
Figure 5.28: Bubble elongation for different viscosity ratios $\lambda$, Re=10, Ca=0.2
Chapter 6

Conclusions

A volume-of-fluid method using the PISO algorithm [20] has been used to investigate the
deformation and breakup of bubbles in a centimeter-scale T-junction.
Bubbles in high confinement show a slight increase in stability compared to bubbles in
non-confined geometries. If the purpose is to reduce possibility of breakup, localizing the
boundaries far away from the bubble motion is preferred. The analysis shows three different
breakup regimes for the Reynolds number range studied: the non-breakup regime, where the
motion of the flow is not enough to break the bubble apart and it remains attached to the
bottom wall of the T-junction; the first breakup regime, where the bubble is stretched and
elongated due to the motion of the flow before reaching the bottom wall causing a breakup
of the original bubble into a large secondary bubble and a remaining satellite that eventually
leaves the T-junction through the outlets; and the second breakup regime, where the breakup
results again into a large bubble and a satellite. However, before the breakup the bubble
suffers some deformation into a crown-shaped bubble that eventually breaks. The first
breakup regime is more widely found for most of the Reynolds numbers, Capillary numbers
and viscosity ratios analyzed. The boundaries between these regimes depend strongly on
the Re-Ca combination. Changing the viscosity ratio affects these boundaries in the Re-Ca
chart. Figure 6.1 shows the boundaries for the three regimes depending on the viscosity
ratio.
Results for different Reynolds numbers show how the bubble suffers a deceleration for larger Re numbers in the first breakup regime until the bubble transitions into the second breakup regime, where it suddenly accelerates and produces a fast breakup. Larger breakup times lead to larger breakup distances, as expected. Low Re numbers do not result in deformation since the inertia of the flow is not sufficient to overcome the interface forces. Results for low capillary numbers show good agreement with other investigations, numerically [9] and experimentally [12]. Bubble deformation and elongation are particularly sensitive to changes in surface tension. Large values of surface tension prevent bubble breakup even though walls of the geometry are encountered rapidly, as expected. Increasing the capillary number results in a more significant deformation and elongation. This elongation can be so long that the deformed bubble does not break even after crossing the outlets. The first breakup regime is more commonly found for most of the capillary numbers studied. Breakup time and location differ, allowing for a second bubble to split from the original one.

Viscosity ratio is an important parameter for the control of the bubble breakup. Different
viscosity ratios lead to different breakup regimes for equal Re and Ca numbers. Decreasing the viscosity ratio from the base case ($\lambda = 0.01$) extends the first breakup regime and the second breakup regime. On the contrary, increasing the viscosity ratio expands the first breakup regime, becoming even more common.
Bibliography


