CFD Simulations of Macroscopic and Microscopic Multiphase Fluid Flow and Droplet Interaction

Aaron Harrington
Louisiana State University and Agricultural and Mechanical College

Follow this and additional works at: https://repository.lsu.edu/gradschool_theses

Part of the Transport Phenomena Commons

Recommended Citation
https://repository.lsu.edu/gradschool_theses/5471

This Thesis is brought to you for free and open access by the Graduate School at LSU Scholarly Repository. It has been accepted for inclusion in LSU Master's Theses by an authorized graduate school editor of LSU Scholarly Repository. For more information, please contact gradetd@lsu.edu.
COMPUTATIONAL FLUID DYNAMICS SIMULATIONS OF MACROSCOPIC AND MICROSCOPIC MULTIPHASE FLUID FLOW AND DROPLET INTERACTION

A Thesis

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Master of Science

in

The Gordon A. and Mary Cain Department of Chemical Engineering

by

Aaron Craig Harrington
B.S., University of Florida, 2008
December 2021
Acknowledgements

First I would like to thank both Dr. Nandakumar and Dr. Benton. Your guidance has been invaluable even if it was difficult for me to keep up.

I would also like to thank, in general, the faculty and staff of the Department of Chemical Engineering at LSU. Everyone here has made this place feel like a second home.

I would also like to thank my fellow graduate students in the department, past and present who have become some of my closest friends here.

And finally I would like to dedicate this dissertation to my daughter, Giselle, who’s arrival in my life has made the journey and the struggle worthwhile.
# Table of Contents

Acknowledgements ............................................................................................................................... ii

Abstract ........................................................................................................................................................... v

Chapter 1. General Information .................................................................................................................. 1
  1.1. Computational Fluid Dynamics (CFD) Models ................................................................................. 1

Chapter 2. Euler-Euler Method for Modeling Liquid-Gas Flow ................................................................. 4
  2.1. Euler-Euler Model ............................................................................................................................. 4
  2.2. Turbulence Modeling ......................................................................................................................... 4
  2.3. Interfacial Forces ............................................................................................................................... 5

Chapter 3. Subcooled Boiling Multiphase Flow ......................................................................................... 7
  3.1. Introduction .......................................................................................................................................... 7
  3.2. Literature Review .............................................................................................................................. 7
  3.3. Numerical Modeling .......................................................................................................................... 15
  3.4. Simulation Setup ............................................................................................................................... 22
  3.5. Results and Discussion .................................................................................................................... 24
  3.6. Conclusions ....................................................................................................................................... 34

Chapter 4. Volume of Fluid Method for Modeling Droplet Interaction ...................................................... 36
  4.1. Volume of Fluid Method ..................................................................................................................... 36

Chapter 5. Microfluidic Droplet Generation and Interaction ...................................................................... 38
  5.1. Introduction .......................................................................................................................................... 38
  5.2. Literature Review .............................................................................................................................. 38
  5.3. Droplet Generation ............................................................................................................................. 48
  5.4. Three Phase System Test .................................................................................................................. 56
  5.5. Numerical Model ............................................................................................................................... 63
  5.6. Results and Discussion .................................................................................................................... 69
  5.7. Conclusions ....................................................................................................................................... 77

Chapter 6. Summary ...................................................................................................................................... 78
  6.1. Subcooled Boiling Multiphase Flow ................................................................................................. 78
  6.2. Liquid-Liquid Droplet Generation and Interaction ........................................................................ 78

Appendix A. Equations and constants used in turbulence modeling, Chapter 2 ..................................... 79
Abstract

Multiphase flow is a complex phenomenon which can be modeled on numerous different length scales, both macroscopically and microscopically.

The use of a Euler-Euler model for Computation Fluid Dynamics (CFD) simulations of subcooled boiling phenomena is discussed in detail. The CFD conditions have been set up to mimic previous experimental conditions. A cylindrical vessel with subcooled liquid flow is heated along part of the axial wall of the vessel. A constant heat flux is applied to produce subcooled boiling. We discuss the development of the phase change within the vessel as well as the temperature profile, and validate the results with respect to the experimental setup.

We then look at the development of stable non-coalescing droplets, in a microfluidic simulation. It is difficult to develop a computational method which can create stable droplets which interact with one another without coalescence. In order to understand the operating conditions of dilute droplet flow without coalescence we adopt a method of phase identification in the volume of fluid method that allows for droplets of the same phase to interact with each other while preventing coalescence. We then examine the properties of droplet formation and propagation in a diverging/converging microchannel in a dilute droplet regime. We demonstrate the link between droplet size and flowrate can be controlled and also that simulated droplet propagation and interaction agrees with experiment.
Chapter 1. General Information

The phrase multiphase flow is used to describe a general system where there are two or more distinct thermodynamic phases flowing simultaneously. These configurations can take several forms, from simple flows of two immiscible liquids to complicated patterns involving liquid, gas, and in some cases even solid flows. Multiphase flow patterns exist in all forms in nature and industry, from the flowing sediment of river deltas to the inner workings of a distillation column.

Generally speaking there are two categories of flow—dispersed flow and separated flow. In dispersed flow, finite droplets are distributed throughout a continuous phase of a medium. In separated flow is characterized by continuous streams of fluids which are separated via interfaces. This dissertation will examine specific situations from both of these categories.

In the first instance we will examine a gas-liquid dispersed flow incorporating phase change. Specifically a system with two regimes; one where subcooled nucleate boiling occurs and a separate regime where film condensation occurs.

In the second instance we will examine a liquid-liquid separated flow in which the system produces large droplets and is able to describe the droplet-droplet interactions.

1.1. Computational Fluid Dynamics (CFD) Models

Historically, attempting to model multiphase flows was done via empirical correlations, one- or two dimensional models, or simplified single-phase analysis with corrective terms. These models attempt to demonstrate a relationship connecting the multiphase flow patterns to the configuration of the system in question. Difficulty would always arise for situations with non-spherical geometry, or situations where the mass transfer coefficients were either unknown or required fitting to the specific problem in question. In all cases, the models were unable to
take into account any specific details, and were not able to analyze the flow on levels that would give deep insight into the workings of complex mixtures and flow patterns.

The increase in computational power over the last two decades has given rise to the development of more robust numerical models, which has facilitated the development of computational fluid dynamics to be a viable tool in modeling systems of increasing size, scale, and complexity. Full three dimensional models are possible and fine grain details incorporating such phenomena and turbulence can be modeled and studied with great accuracy.

Figure 1.1 shows the hierarchy of modeling techniques available and the range of such models depending on the length scale of the phenomena one is attempting to simulate.

The methods of interest for us are the Euler-Euler method and the Volume of Fluid method. In the Euler-Euler method[1], the two phases (in our case, a dispersed gas in a liquid)
are treated as an interpenetrating continuum. Each phase has its own set of governing equations, and while this allows for detailed analysis and construction of interpenetrating forces, it can be computationally expensive. In the Volume of Fluid method (VOF)\cite{2} the simulation tracks the fraction of the computational cell of interest that is occupied by the fluid. This data is then used to construct the interface between the fluids. It has been shown to accurately model surface and interface phenomena, but fails when it comes to physics of droplet-droplet interactions of the same fluid in a continuous media. We have taken a novel computational approach to allow for droplet-droplet interaction in a VOF simulation at minimal computational expense.

In Chapter 2 we will touch on the Eulerain-Eulerian model as well as discuss the k-ω turbulence model as well as the various interfacial forces that will be used in the model.

In Chapter 3 we present the modeling of a system of subcooled wall boiling and thin film condensation. The Euler-Euler model is employed along with a subcooled boiling model and phase change mechanism, which are discussed in this chapter. The results of the simulation are compared and validated against experimental data.

In Chapter 4 we discuss the VOF method and laminar liquid-liquid flows as well as interface tracking and droplet generation.

In Chapter 5 we use a VOF model to simulate droplet generation in a liquid-liquid multiphase flow under laminar conditions. A novel modification to the simulation code is employed to allow for the interaction of droplets of the same physical properties, normally not possible using the VOF method.

And in Chapter 6, we summarize the work.
Chapter 2. Euler-Euler Method for Modeling Liquid-Gas Flow

The modeling of systems in which one phase is dispersed into another, typically liquid-gas flows here the gas is dispersed into the liquid, is typically done in what is called an Euler-Euler framework. In this schema, one phase (typically the liquid phase) is described as the continuous phase, and the other phase (gas) is described as the dispersed phase. This model treats each phase as independent, with its own set of governing equations, and those equations contain terms related to the interfacial forces between the two phases.

2.1. Euler-Euler Model

In order to derive the governing equations for the interactions, we treat the dispersed gas phase as a continuum, with all the interactions between the phases being contained in the momentum equation. These equations also account for the mass transfer that can occur during phase change. We therefore have a total of two continuity equations (2-1) and two momentum equations (2-2), one set for each phase. The pressure and velocity coupling is determined by the SIMPLE algorithm [3]

\[
\frac{\partial}{\partial t} (\alpha_a \rho_a) + \nabla \cdot (\alpha_a \rho_a \vec{u}_a) = \sum_{b=1}^{n} \Gamma_{ab}
\]

(2 - 1)

\[
\frac{\partial}{\partial t} (\alpha_a \rho_a \vec{u}_a) + \nabla \cdot (\alpha_a (\rho_a \vec{u}_a \times \vec{u}_a)) =
\]

\[
= -\alpha_a \nabla p + \nabla \cdot (\alpha_a \mu_a (\nabla \vec{u}_a + (\nabla \vec{u}_a)^T)) + \sum_{b=1}^{n} (\Gamma_{ab}^+ \vec{u}_b - \Gamma_{ba}^+ \vec{u}_a) + F_a
\]

(2 - 2)

2.2. Turbulence Modeling

Two-equation turbulence formulations have been shown to provide a reasonable compromise between computational cost and accuracy. For the purposes of these simulations, the turbulence velocity scale is determined based on the turbulent kinetic energy, which is based on
the solution to the turbulence equations. The k-ω Shear Stress Transport (SST) model was chosen based on its ability to more accurately model turbulent forces in near-wall environments.

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k U_i) = \frac{\partial}{\partial x_i} \left( \left( \mu + \frac{\mu_t}{\sigma_{k3}} \right) \frac{\partial k}{\partial x_i} \right) + P_k - \beta' \rho k \omega + P_{kb} \tag{2-3}
\]

\[
\frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial x_i} (\rho \omega U_i) = \frac{\partial}{\partial x_i} \left( \left( \mu + \frac{\mu_t}{\sigma_{\omega3}} \right) \frac{\partial \omega}{\partial x_i} \right) + \frac{(1 - F_1) 2 \rho}{\sigma_{\omega2} \omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i} + \frac{\alpha_3}{k} \omega P_k - \beta_3 \rho \omega^2 + P_{\omega b} \tag{2-4}
\]

where,

\[\mu_t = \frac{\rho k}{\omega}\] (2-5)

A detailed description of the various constants and blending functions used in turbulence calculations can be found in Appendix A.

2.3. Interfacial Forces

The drag force of the liquid exerted on the gas, with the description given by Ishii\[4\] where

\[F_{\text{drag,ab}} = -\frac{3}{4} \frac{C_D}{d} \rho_a \alpha_b |\vec{u}_b - \vec{u}_a| (\vec{u}_b - \vec{u}_a)\] (2-6)

with the drag coefficient, \(C_D\), being determined by\[5\]

\[C_{D,\text{sphere}} = \max \left( \frac{24}{Re} \left(1 + 0.1Re^{0.75}\right), 0.44 \right) \tag{2-7}\]

\[C_{D,\text{cap}} = \frac{8}{3} \tag{2-8}\]

\[C_{D,\text{ellipse}} = \frac{2}{3} \sqrt{Eo} \tag{2-9}\]

\[Eo = \frac{g (\rho_l - \rho_g) d_p^2}{\sigma} \tag{2-10}\]

\[C_D = \max (C_{D,\text{sphere}}, \min (C_{D,\text{ellipse}}, C_{D,\text{cap}})) \tag{2-11}\]
The lift force is incorporated via the formulation:

\[ F_{lift,a} = -C_l \rho_a \alpha_a (\vec{u}_b - \vec{u}_a) \times (\nabla \times \vec{u}_a) \quad (2 - 12) \]

where the lift coefficient, \( C_l \), is determined by

\[ C_l = \begin{cases} \min(0.288 \tanh(0.121Re), f(Eo_{\perp})) & Eo_{\perp} < 4 \\ f(Eo_{\perp}) & 4 < Eo_{\perp} < 10 \\ -0.27 & 10 < Eo_{\perp} \end{cases} \quad (2 - 13) \]

with

\[ f(Eo_{\perp}) = 0.00105Eo_{\perp}^3 - 0.0159Eo_{\perp}^2 - 0.0204Eo_{\perp} + 0.474 \quad (2 - 14) \]

\[ Eo_{\perp} = \frac{g(\rho_l - \rho_g)d_{\perp}^2}{\sigma} \quad (2 - 15) \]

\[ d_{\perp} = d_p \sqrt[3]{1 + 0.163Eo^{0.757}} \quad (2 - 16) \]

And finally, the turbulent dispersion force was incorporated[6]

\[ \vec{F}_{td,a} = -\frac{3\alpha_a}{4d_p}(\vec{u}_b - \vec{u}_a) \frac{\mu_{TD}}{\sigma_{TD}} \left( \frac{1}{\alpha_b} + \frac{1}{\alpha_a} \right) \nabla \alpha_a \quad (2 - 17) \]
Chapter 3. Subcooled Boiling Multiphase Flow

3.1. Introduction

This chapter explores the modeling of the phenomena of subcooled boiling. The CFD conditions have been set up to capture the conditions studied experimentally[7]. In this simulation we have a cylindrical vessel with mass flow inward and a heated section along part of the axial wall of the vessel. A constant heat flux is applied to produce subcooled boiling. We discuss the development of the phase change within the vessel as well as the temperature profile, and validate the results with respect to the experimental setup.

3.2. Literature Review

3.2.1. Subcooled Wall Boiling

Wall Boiling is a physically complex process in which energy, momentum and mass transfer between a solid wall and single and two-phase fluid is coupled. Since the 1950s, various models have been proposed and developed to more accurately predict the rate of heat transfer that occurs in a system which undergoes subcooled boiling. Generally speaking, these models fall into one of three categories: the first can be described as determining the wall heat via empirical correlations, the second are empirical correlations for determining the wall heat flux contribution from the liquid and vapor phases. And the third constitute models which outline mechanisms for both the wall heat flux and the contribution to the flux from each individual phase. The first category, wall heat flux correlations are quite limited and will usually only be applicable for a specific flow configuration. They are the result of purely empirical measurements that has been gathered over the course of several experiments. They do not provide any insight into which phase or mechanism contributes to the heat flux in a given manner. In order to accurately model this process, we consider the wall boiling as a nucleation
phenomenon. Nucleation is the initial step in the process of forming a new thermodynamic phase, in this case, the formation of vapor from liquid. On the macroscopic level, however, nucleation is a stochastic process, so we must devise an appropriate model to reflect the microscopic process in a macroscopic system. Once nucleation has begun, for any given bubble, the bubble grows via evaporation of the liquid at the liquid-vapor interface.
In order to accurately model boiling phenomena we must first describe the theory of heat and mass transfer in a two phase system. Since Wall Boiling is a process of nucleated boiling, we must devise a theory on how to accurately model a fundamentally atomic and microscopic phenomenon in the macroscopic continuum. Since empirical models lack the ability to tell us how the process occurs, phenomenologically, we turn to mechanistic models; which look at individual heat transfer mechanisms that occur during phase change and can contribute to the overall heat flux. Therefore, a mechanistic model can tell us both the overall heat flux as well as the heat flux contribution from the vapor and liquid phases respectively.

A conceptual subcooled boiling system is depicted in Figure 3.1. Subcooled liquid enters the vessel at the inlet, the vessel with heated surfaces. Downstream, when the wall temperature has reached a critical value, nucleation begins to occur. Further downstream, the nucleated bubbles are small and still adhering to the heated wall, however, they being to grow the further downstream one goes. As the temperature in the bulk liquid increases, the bubbles will detach from the nucleation sights and migrate downstream with the flow. The vapor fraction begins to increase rapidly after this point.

Figure 3.2 is a flow boiling curve. Like the general scheme of Figure 3.1 it consists of three regimes, a region dominated by forced convection in the bulk fluid, a region of partial boiling, and fully developed boiling. Prediction of this curve is the goal of any model of heat transfer. We are going to explore the partial and fully developed regions in this review.
Some of the first attempts as modeling partial nucleate boiling were done[8], using a superposition model to calculate the nucleate boiling heat flux

\[ q_{pb} = q_{fc} + q_{nb} \quad (3 - 1) \]

where \( q_{nb} \) is pool boiling heat flux, \( q_{fc} \) is the single phase heat flux, and \( q_{pb} \) is the heat flux during partial boiling. Examining the curves for both the single phase and the fully developed boiling, the heat flux at the intersection of those curves can be used to determine the point where fully developed nucleate boiling begins. Additionally, this model the heat flux in the single phase region was calculated via

\[ q_{fc} = h_{fc} (T_{sat} - T_i) = h_{fc} \Delta T_{sub} \quad (3 - 2) \]

where the heat transfer coefficient \( h_{fc} \) is calculated using typical correlations. While this model provides for a way to begin to understand the heat flux contributions from the various phases, it
is simple and does not reflect many of the factors that come into play in more complicated two phase flow.

Additional formulae were proposed to attempt to calculate the various heat transfer coefficients that correspond to the regions of different heat flux such as[9],

\[ h_{pb} = \sqrt{h_{fc}^2 + h_{nb}^2} \]  \hspace{1cm} (3 - 3)

\( h_{nb} \) is the fully developed boiling heat transfer coefficient for

\[ h_{nb} = C(p)q_w^{0.7} \]  \hspace{1cm} (3 - 4)

and \( C(p) \) is a pressure based function.

The fully developed nucleate boiling curve is given as

\[ q_{nb} = \mu_l h_{fg} \sqrt{g(\rho_l - \rho_g)} Pr_l^{-m/n} \left( \frac{C_{p,l}(T_w - T_{sat})}{C_s h_{fg}} \right)^{1/n} \]  \hspace{1cm} (3 - 5)

where \( C_s, m \) and \( n \) are empirical constants.

3.2.2. Nucleate Boiling.
There have also been correlations developed for the heat flux for fully developed nucleate boiling. One of the earliest was a power law relationship [10]

\[ q_{fd} = C_2(\Delta T_w)^{3.86} \]

where \( C_2 \) is an empirical constant. The theme of a power law as a function of the temperature difference between the wall and the bulk would be repeated [11,12]

\[ q_{fd} = \left( e^{p/62} \frac{\Delta T_w}{25} \right)^4 \]  \hspace{1cm} (3 - 6)

\[ q_{fd} = \left( e^{p/87} \frac{\Delta T_w}{22.65} \right)^2 \]  \hspace{1cm} (3 - 7)

\[ q_{fd} = \left[ 1058(\dot{m}h_{fg})^{0.7} F_f h_{lo}(\Delta T_w + \Delta T_{sub})^{1/0.3} \right]^{1/0.3} \]  \hspace{1cm} (3 - 8)

3.2.3. Wall Heat Flux

Several models have been developed that attempt to correctly predict the partitioning of the wall heat flux. The main differences in these models are which physical mechanisms are proposed and the degree to which they attribute the total heat to each individual mechanism. One of the first models was based on empirical observation of the presence of two regions, a region with low temperature and very small bubbles, and then a region with higher temperature where
larger bubbles had formed and become detached. The heat flux equation was divided into two components: into single phase and boiling

\[ q_w = q_{fc} + q_b \]  \hspace{1cm} (3\textendash9)

The boiling heat flux was set equal to the condensation heat flux such that

\[ q_c = q_b = q_w - q_{fc} = B_0 h_{fc} \frac{A_c}{A_h} \Delta T_{sub} \]  \hspace{1cm} (3\textendash10)

This simplified to

\[ q_c = \frac{B_1 \alpha w h_{fc}^2 \Delta T_{sub}}{k_l P \eta_l} \]  \hspace{1cm} (3\textendash11)

where \( B_1 \) is a constant. Here, in the area of low temperature, the condensation from the bubbles acts as a separate path for the heat transfer from the wall into the bulk fluid. The model therefore assumes that all the heat transferred into the liquid in the region goes into heating the bulk liquid and not to any nucleation phenomena.

In developing a model for nucleated boiling, we choose to use the Rensselaer Polytechnic Institute, or RPI boiling model.

3.2.4. RPI Boiling Model

The phenomena of subcooled boiling occurs when a bulk liquid below saturation temperature is in contact with a wall which is slightly above the liquid’s saturation temperature. This contact between the relatively cold fluid and hot wall causes heat to transfer to the fluid, but
not in such quantities as to cause a phase change in the bulk. Rather it is the situation where liquid which is entrenched in micro cracks within the wall’s surface (since in general, no surface is perfectly smooth) causes the heat to be transferred to a small amount of liquid directly on the surface. This mass of liquid undergoes phase change and then forms a vapor bubble on the surface. This bubble grows until it is large enough that the forces of surface tension (and possibly bulk fluid movement) cause it to detach from the wall. This process is call nucleation. Nucleation is a stochastic process, and thus difficult to model explicitly. Various methods are discussed including partial nucleate boiling, fully developed nucleate boiling and the various models for partitioning the wall heat flux in order to accurately model the phenomenon. They detail several mechanistic models which each use different formulations to express the components of the heat flux. One model used to predict wall boiling is the RPI boiling model[13]. The model describes the process of nucleation using the subcooled, superheat, and saturation temperatures of the system. It breaks up the heat flux at the wall into three components, quantifying the contribution to the heat flux from the phenomena of convection, evaporation, and quenching.

There are several different iterations of the RPI model, each with their own closure equations, making various assumptions. Additionally, in order to close the model, different schemes for determining vapor bubble diameter have been included, usually determining bubble diameter based on liquid subcooled temperature or on a population balance based on coalescence and breakup after wall departure.

Various experiments have been conducted in order to study the phenomena of subcooled boiling[7,14]. They have been designed under laboratory conditions so that the experimental set up has dimensionless parameters which mimic the dimensionless parameters of various industrial applications. Therefore the model and simulations should scale appropriately to different
applications, given that the dimensionless phenomena remain comparable.

3.3. Numerical Modeling

The system for modeling both subcooled boiling and thin film condensation requires that we add in the energy equation as well as mass transfer terms to the Euler-Euler model discussed in Chapter 2. Additionally, we must define the models used to capture the mass transfer phenomena as a function of temperature.

3.3.1. Thermal Modeling

The governing equations for modeling of the reflux are developed in a Euler-Euler framework. In addition to the mass and momentum governing equations discussed in Chapter 2, due to the existence of temperature gradients and phase change, we introduce the energy equation for each individual phase:

$$\frac{\partial}{\partial t} \left( \alpha_a \rho_a h_a \right) + \nabla \cdot \left( \alpha_a \rho_a \bar{u}_a h_a \right) =$$

$$= \alpha_a \frac{\partial p_a}{\partial t} + \nabla \cdot \left( \alpha_a \lambda_a \nabla T_a \right) + \alpha_a \nabla \cdot \left( \bar{u}_a \cdot \bar{e}_a \right) + Q_a + \sum_{b=1}^{n} \left( \Gamma_{ab}^+ h_b - \Gamma_{ba}^+ h_a \right)$$

(3 - 12)

with the liquid heat transfer coefficient described by[15]

$$h_{\text{L,G}} = \frac{k_L}{d_p} Nu = \frac{k_L}{d_p} \left( 2 + 0.6 Re^{1/2} Pr^{1/3} \right)$$

(3 - 13)

3.3.2. Boiling Modeling

In developing a model for nucleated boiling, the project uses the model known as the RPI boiling model (developed at Rensselaer Polytechnic Institute). This is a mechanistic model
developed to macroscopically model the phenomenon of nucleation based on superheat and subcooled temperatures of the wall and fluid at the wall, respectively.

The source term added to the energy equation is divided into three parts to represent the three different mechanisms.

\[ Q_T = Q_c + Q_e + Q_q \]  \hspace{1cm} (3 - 14)

Here, \( Q_c \) refers to the heat transferred to the liquid due to normal convective heat transfer into the fluid. \( Q_e \) is the heat transfer into the evaporated vapor phase of the bubble, while the bubble is growing, before detachment. \( Q_q \) is the heat transfer at the wall due to the quenching phenomenon, where after the bubble has detached, cold liquid will flow back over the nucleation site at the wall. Since the fluid is either subcooled or at saturation conditions and the vapor bubble assumed to be at saturation temperature, this fluid will always be at most the same temperature as the bubble, and will therefore produce a "cooling" or "quenching" effect at the wall.

The heat transfer due to convection is determined by

\[ Q_c = (1 - A_W)h_c(T_W - T_L) \]  \hspace{1cm} (3 - 15)

Where \( h_c \) is given by

\[ h_c = \frac{\rho C_p \mu_T}{T^+} \]  \hspace{1cm} (3 - 16)

The above equation is a reformulation of the conventional definition of the heat transfer coefficient, \( \frac{q}{\Delta T} \), using substitution based on the logarithmic “law of the wall”

\[ u^+ = \frac{1}{\kappa} \ln y^+ + C^+ \]  \hspace{1cm} (3 - 17)
There we see \( h_c \) is scaled based on a dimensionless temperature, \( T^+ \). This temperature corresponds to the temperature at a certain distance \( y^+ \), where the \( y^+ \) and \( T^+ \) terms are defined as follows:

\[
\begin{align*}
    u_\tau &= \sqrt{\frac{\tau_w}{\rho}} \quad (3-18) \\
    u^+ &= \frac{u}{u_\tau} \quad (3-19) \\
    y^+ &= \frac{yu_\tau}{v} \quad (3-20) \\
    T^+ &= \frac{T_W - T}{T_\tau} \quad (3-21) \\
    T_\tau &= \frac{q_w}{\rho C_p u_\tau} \quad (3-22)
\end{align*}
\]

From the above equations, we can see that the \( y^+ \) term corresponds to the logarithmic position as determined by the law of the wall. In this way, the wall shear stress and the analogy between momentum and heat transfer plays an important part in determining the heat transfer coefficient.

The heat transfer due to evaporation is given by

\[
\begin{align*}
    Q_E &= \dot{m}_w H_{LG} \quad (3-23) \\
    \dot{m}_w &= \rho_g \frac{\pi}{6} d_w^3 f N \quad (3-24)
\end{align*}
\]

Where \( \dot{m}_w \) is the mass flow rate, \( d_w \) is the bubble departure diameter, \( f \) is the bubble departure frequency and \( N \) is the nucleation site density. These terms are derived based on empirical correlations based on the temperature gradients relative to saturation temperature of the system. \( d_w \) is the bubble departure diameter, which is the size of the bubble as it leaves the wall. Its growth is based on the local liquid subcooling as presented in the following empirical equation.
Here, \( d_{\text{ref}} \) is an empirical parameter. Similarly, the nucleation site density is defined as the local wall superheat with the equation

\[
N = N_{\text{ref}} \left( \frac{T_W - T_L}{\Delta T_{\text{ref}N}} \right)^p
\]  

(3 – 26)

The nucleation site density is the number of individual nucleation sites within a given area on the wall, and is dependent on the wall superheat. Bubble departure frequency is a measure of how often a fully formed bubble detach at any given nucleation site and begin flowing along with the bulk fluid.

\[
f = \sqrt{\frac{4g(\rho_L - \rho_G)}{3d_W \rho_L}}
\]  

(3 – 27)

It is based on the density difference between the liquid and vapor, as well as the vapor bubble departure diameter at that particular nucleation site.

Quenching, \( Q_Q \), is defined as

\[
Q_Q = A_W h_Q (T_W - T_L)
\]  

(3 – 28)

With \( h_Q \) being

\[
h_Q = \frac{2}{\sqrt{\pi}} f \sqrt{\frac{t_{\text{wait}} k_L \rho_L C_{pL}}{t_{\text{wait}} k_L \rho_L C_{pL}}}
\]  

(3 – 29)

\( h_Q \) is based on the analytical solution to the 1-D transient condition problem[16]. However, \( t_{\text{wait}} \) is an empirical parameter defined as the time between one bubble departing and another forming at any given nucleation site, which is only accurate where the heat flux on the wall is at least 75% of the critical heat flux[17].

\[
t_{\text{wait}} = \frac{0.8}{f}
\]  

(3 – 30)
In both the expressions for $Q_c$ and $Q_q$ we have a term $A_w$ which is the area influence factor, defined as

$$A_w = \pi \left( a \frac{d_w}{2} \right)^2 N$$  \hspace{1cm} (3 - 31)

The area influence factor is a measure how much of the pipe wall exposed to fluid is "under the influence" of bubbles. It should be known that the area influence factor must remain small for the model to be valid. As $A_w$ approaches 1, the system is approaching critical heat flux, where the model breaks down and another must be employed.

As boiling occurs, the vapor bubble will move away from the wall and, due to the turbulence inherent in the system and two phase interaction, migrate into the bulk. Bubble diameter in the bulk is based on an empirical correlation between size and local subcooled temperature.

3.3.3. Population Balance Modeling (PBM)

In order to better model the phenomena in the pipe, we attempt to model the bubble diameter of the dispersed phase not as a function of local subcooled temperature, but as a population balance of individual bubbles of a given diameter, modeling both coalescence of smaller bubbles into larger ones and breakup of larger bubbles into smaller ones.

The MUSIG (Multiple Size Group) model places particles, or bubbles, into discrete groups, called bins, based on specific criteria, be it mass or diameter. A number density is associated with each bin to signify how many bubbles can be said to occupy a particular bin. Bubbles can move, via a defined mechanism, from one bin to an adjacent bin. Such a model can be homogeneous or inhomogeneous depending on how the velocity vector is applied to the model. In the homogeneous MUSIG model, the velocity vector of a given numerical cell is
applied to all classes of bins in the system. In Inhomogeneous MUSIG, each bin, or possibly

group of bins, has its own velocity term.

The MUSIG model that has been integrated into ANSYS CFX. It provides a framework
for the integration of population balance into three dimensional CFD calculations.

The MUSIG model begins with the population balance equation, which is a balance
equation of the number density of particles of a given mass at a given time

$$\frac{\partial}{\partial t} n(m, t) + \frac{\partial}{\partial x_i} \left( U^i(m, t) n(m, t) \right) = B_B - D_B + B_C - D_C$$

where the source terms on the right hand side of the equation correspond to: the birth of bubbles
of a given size due to the breakup of larger bubbles; the death of bubbles due to their breakup
into smaller bubbles; and the birth of this size bubble due to coalescence of smaller bubbles; and
finally the death of bubbles due to their coalescence into larger sized bubbles.

These terms are functions of the specific breakup rate $g(m; \varepsilon)$ and specific coalescence rate
$Q(m; \varepsilon)$, where bubbles of mass $m$ are breaking up into bubbles of mass $\varepsilon$ and $m-\varepsilon$ and bubbles
of mass $m$ and $\varepsilon$ are coming together to form bubbles of mass $m+\varepsilon$, respectively.

$$B_B = \int_{m}^{\infty} g(\varepsilon; m)n(\varepsilon, t) \, d\varepsilon$$

$$D_B = n(m, t) \int_{0}^{m} g(\varepsilon; m) \, d\varepsilon$$

$$B_C = \frac{1}{2} \int_{0}^{m} Q(m - \varepsilon; \varepsilon)n(m - \varepsilon, t)n(m, t) \, d\varepsilon$$
\[ D_C = n(m, t) \int_0^\infty Q(m; \varepsilon) n(\varepsilon, t) \, dt \]  

The specific breakup and coalescence models available were the Lou and Svendsen model for breakup and the Prince and Blanch Model for coalescence. A detailed breakdown of these models can be found in Appendix 3.

When determining the criteria for the distribution of bins, we take into consideration the fact that droplet diameter is the most important factor for the bubbly flow. The relationship between bubble mass and diameter is determined via equation 3-37 and the diameters of the various bins are determined via the formulas in equations 3-38 and 3-39.

\[ m = \rho_G \frac{\pi d^3}{6} \]  

\[ d_i = d_{\text{min}} + \Delta d \left( i - \frac{1}{2} \right) \]  

\[ \Delta d = \frac{d_{\text{max}} - d_{\text{min}}}{N} \]

\[ d_{\text{min}}, d_{\text{max}}, \text{ and } N \] being the minimum bubble diameter, maximum bubble diameter, and the number of groups, respectively.
3.4. Simulation Setup

The simulation was designed to model the geometry of the DEBORA experiments[7] in order to validate the boiling model under flow and phase change conditions. The DEBORA experiments were a series of experiments examining the boiling of Freon R12 under specific conditions. These conditions were chosen in order to mimic the dimensionless parameters that might be found on large Pressure Water Reactors in order to help with the design and implementation of water flowing in heated tubes as it approaches critical heat flux. The radial properties of vapor hold up, liquid temperature and liquid and vapor velocity were gathered for a series of experiments, representing parametric studies with regards to heat flux, liquid temperature, and liquid velocity.

The experimental set up is as follows: fluid flows against gravity into a vertical pipe, at a temperature below saturation conditions, along the length of which a constant heat flux is applied. The system, is modeled as a 2.5D pipe-wedge with an inner radius of 0.0096 m and a length of 3.5 m. Symmetry conditions are applied alone the faces of the wedge. The heat flux applied along the wall is 73.89 kW/m². Table 3.1 gives a list of the system properties in the simulations and a sketch of the geometry wedge can be seen in Figure 3.2.
Table 3.1. Simulation System Properties

<table>
<thead>
<tr>
<th>System Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat flux [W m$^{-2}$]</td>
<td>7.5x10$^4$</td>
</tr>
<tr>
<td>Liquid viscosity [kg m$^{-1}$ s$^{-1}$]</td>
<td>89.5 x 10$^6$</td>
</tr>
<tr>
<td>Mass flux [kg m$^{-2}$ s$^{-1}$]</td>
<td>2x10$^3$</td>
</tr>
<tr>
<td>Liquid specific heat capacity [J kg$^{-1}$ K$^{-1}$]</td>
<td>1.42 x 10$^3$</td>
</tr>
<tr>
<td>Characteristic pipe diameter [m]</td>
<td>0.02</td>
</tr>
<tr>
<td>Liquid Density [kg m$^{-3}$]</td>
<td>1.02 x 10$^3$</td>
</tr>
<tr>
<td>Vapor Density [kg m$^{-3}$]</td>
<td>0.172 x 10$^3$</td>
</tr>
<tr>
<td>Characteristic fluid velocity [m s$^{-1}$]</td>
<td>1.96</td>
</tr>
<tr>
<td>Liquid specific heat capacity [J kg$^{-1}$ K$^{-1}$]</td>
<td>1.42 x 10$^3$</td>
</tr>
<tr>
<td>Characteristic fluid velocity [m s$^{-1}$]</td>
<td>1.96</td>
</tr>
<tr>
<td>Enthalpy of Vaporization [J kg$^{-1}$]</td>
<td>293 x 10$^3$</td>
</tr>
<tr>
<td>Liquid thermal conductivity [W m$^{-1}$ K$^{-1}$]</td>
<td>0.0457</td>
</tr>
<tr>
<td>System Pressure [MPa]</td>
<td>2.62</td>
</tr>
</tbody>
</table>

Figure 3.2. System geometry for subcooled boiling domain
3.5. Results and Discussion

3.5.1. Mesh Independence

Mesh independence tests were performed varying the mesh size in both the radial and axial pipe directions. Although the mesh remained uniformly distributed in the axial direction throughout the simulations, the element size in the radial direction was varied in order to create a finer mesh within the boundary layer near the wall. Images of two sample meshes can be seen in Figures 3.1 and 3.2. Figure 3.3 shows a comparison of gas volume fractions for various meshes. The details of the meshes being listed in Table 3.2.
It’s important to note that the major difference between the results of the mesh come not from axial refinement, but from boundary layer refinement. In cases where the radial refinement of the mesh is identical, the mesh size in the axial dimension shows almost no difference in vapor holdup, despite having a grid length difference of almost an order of magnitude. This allows a large reduction on computational time since refinement of the boundary layer can be the primary concern for mesh refinement, and axial length can be relatively coarse.

Table 3.2. Mesh Configuration

<table>
<thead>
<tr>
<th>Mesh Number</th>
<th>Radial Refinement</th>
<th>Radial Length (mm)</th>
<th>Axial Length (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Uniform</td>
<td>0.32</td>
<td>8.75</td>
</tr>
<tr>
<td>2</td>
<td>Boundary Layer</td>
<td>0.025 - 1</td>
<td>8.75</td>
</tr>
<tr>
<td>3</td>
<td>Uniform</td>
<td>0.0196</td>
<td>3.5</td>
</tr>
<tr>
<td>4</td>
<td>Uniform</td>
<td>0.192</td>
<td>1.166</td>
</tr>
<tr>
<td>5</td>
<td>Boundary Layer</td>
<td>0.025 - 1</td>
<td>1.166</td>
</tr>
</tbody>
</table>
3.5.2. Validation – Monodispersed model

The CFX simulation is run under steady state conditions. The results are presented as the outlet conditions of the pipe. They are plotted against the experimental results. The gas volume fraction and velocities show reasonable agreement with experiment. Table 3.3 describes the differences between the various DEBORA experiments.

Table 3.3. DEBORA System Properties

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Pressure [MPa]</th>
<th>Mass Flow Rate [kg m(^{-2}) s(^{-1})]</th>
<th>Wall heat flux [kW m(^{-2})]</th>
<th>Inlet Temp [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEBORA 1</td>
<td>2.62</td>
<td>1996</td>
<td>73.89</td>
<td>68.52</td>
</tr>
<tr>
<td>DEBORA 2</td>
<td>2.62</td>
<td>1985</td>
<td>73.89</td>
<td>70.53</td>
</tr>
<tr>
<td>DEBORA 3</td>
<td>1.46</td>
<td>2028</td>
<td>76.2</td>
<td>28.52</td>
</tr>
<tr>
<td>DEBORA 4</td>
<td>1.46</td>
<td>2030</td>
<td>76.24</td>
<td>31.16</td>
</tr>
</tbody>
</table>

For these simulations, the coarse axial grid length was chosen, however the length of the cell was chosen to keep the center of the cell having a corresponding y+ value of approximately 200. This level of refinement is about as good as can be achieved, as at lower values the simulation does not converge.[18] We compare the experimental and simulated results at the
pipe exist for liquid temperature, bubble diameter, gas velocity, and gas fraction for DEBORA 1 and 2. (Figures 3.6 through 3.9)

There is large agreement between simulation and experiment. The largest deviation of simulation from experiment is found in the bubble diameter in the near-wall region. This is because while there is a fitting parameter, it seems that a function in which bubble size is dependent on temperature is not sufficient to correctly capture the full extent of the growth of
bubble size near the wall. Elsewhere in the system, the increased bubble size is likely due to coalescence, but this phenomenon was not modeled.

The bubble diameter being the exception, all other relevant variables have a deviation of no more than 20% of the value, which allows for a reasonable prediction with the current modeling schema. The simulations corresponding to DEBORA 3 and DEBORA 4 were also performed, with this system at a lower pressure (1.46 MPa) than DEBORA 1 and 2. Different
inlet temperatures were used and the overall saturation temperature of the fluid was different because the system pressure was different.

The results for DEBORA 3 and 4 were similar to the results for DEBORA 1 and 2. Deviations for liquid temperature and gas velocity have increased, but not significantly. (Figures 3.10 to 3.13)
It was also investigated whether it was possible to improve the bubble diameter prediction within the framework of the current model. We do so by altering the empirical correlations in the calculation of bubble diameter in the bulk. The effects on the other variables in the system turn out to be negligible, however, the results of bubble diameter distribution do not come closer to matching the experimental results. It is likely that the monodispersed model based on local subcooled temperature is insufficient to capture the phenomenon properly and other techniques should be employed. The discrepancy in bubble diameter between experiment
and the simulation can also be attributed to a deficiency in the modeling of the lift force. Larger bubbles clearly move toward the center of the pipe, and it is likely that a population balance model will be needed to accurately capture this phenomenon.

3.5.3. Validation with PBM

The CFX simulation is run similarly to the trials with monodispersed bubble diameter. Steady state conditions are employed and the results are presented measured from the outlet of the system. The minimum bubble diameter, maximum bubble diameter and number of bins were set to 0 mm, 1.5 mm and 15 respectively. The geometry and mesh used were the same. Here we plot selected results both against the experiment and the monodispersed model for the conditions of DEBORA 1 in Figures 3.14 to 3.17.

In all cases we see some better agreement with experiment and a more robust distribution of the dispersed phase throughout the system. In particular, while the mean bubble diameter is lower than experiment across all radial areas, (compared to the monodispersed simulation where the values were higher than experiment) , the shape of the curve of the bubble diameter distribution more closely resembles that of experiment, especially at the near wall. This suggests that the subcooled boiling model coupled with the population balance model is better able to capture the phenomenon of bubble size distribution, especially in the near wall conditions.

However the overall smallest bubble diameter may be larger than what the model initially predicted. The minimum allowable bubble diameter can be adjusted in the MUSIG model, but this must be compared against nucleation site factors as to what minimum bubble diameter is most reasonable. The gas velocity curve shows better form, but the experiment’s higher value both in velocity and bubble diameter, with a lower gas volume fraction suggest that the simulation does not show the migration and coalescence of larger bubbles to the center of the
pipe as much as occurs in experiment. There may be an issue of bubble development and migration as the system develops, or possibly a limitation with the 2.5-D nature of the simulation.

Overall it appears that while the population balance model is able to better predict the form of the experimental values at the exit, it does not accurately reflect bubble coalescence or initial size at the near wall. This initial under performance likely contributes to the overall lower values across the system.

![Graph](image.png)

Figure 3.14. Debora 1 Comparison of the Gas Volume Fraction at the outlet between experiment and the two simulation models
Figure 3.15. DEBORA 1 Comparison of the Gas Velocity at the outlet between experiment and the two simulation models

Figure 3.16. DEBORA 1 Comparison of the mean bubble diameter at the outlet between experiment and the two simulation models
3.6. Conclusions

A Euler-Euler simulation of two phase flow has been used to model subcooled boiling in a heated pipe. These results were compared against the DEBORA experiments. Bubble diameter and nucleation site density are the two variables which most accurately predict the vapor fraction. While several variables were found to be in good agreement with experiment, the model used to calculate bubble diameter across the radius of the system was found to be inadequate. A population balance model was also employed to investigate the distribution of dispersed phase across the system. While the population balance model was able to better mimic the form of the distribution of variables like gas velocity and mean bubble diameter, it overall under predicted relevant values relative to experiment while the monodispersed model over predicted values. This may be due to issues of radial bubble migration and development in the system. The
Simulation also underpredicts coalescence at the wall which is the likely cause of the lower values overall.
Chapter 4. Volume of Fluid Method for Modeling Droplet Interaction

4.1. Volume of Fluid Method

The volume of fluid (VOF) method is a numerical technique for tracking the interface between fluids. The VOF method can be used for multi-phase systems where the fluids are immiscible. VOF implements and solves a single set of Navier-Stokes equations for the total number of phases present. Each cell in the mesh may contain multiple phases. Using VOF we can simulate all the phases and the interfaces between them as the droplets form and propagate through the channel using a shared velocity field.

A single set of continuity and momentum equations are solved in the computational domain

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \]  

\[ \frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla P + \nabla \cdot [\mu (\nabla \vec{v} + \nabla \vec{v}^T)] + \rho \vec{g} + \vec{F} \]

In addition to the continuity and momentum equations, we introduce the volume fraction of the \( q \)th phase, \( \alpha_q \), in order to allow the VOF method to reconstruct the geometry of the fluid-fluid interface. This requires the use of the advection equation.

\[ \frac{\partial (\alpha_q \rho_q)}{\partial t} + \nabla \cdot (\alpha_q \rho_q \vec{v}) = 0 \]

This volume fraction is also used in equations (1) and (2) in order to calculate the effective density and viscosity of a given cell, based on the volume fraction of the phases present. The volume-averaged density and viscosity, are defined as follows:

\[ \rho = \sum_{1}^{n} \alpha_q \rho_q \]
\[ \mu = \sum_{1}^{n} \alpha_{q} \mu_{q} \]  

(4 - 5)

The additional body force term \( \hat{F} \) in equation (4-2) is computed via the Continuum Surface Force (CSF) model[19], which describes the surface tension forces between the droplet and the continuous fluid.

\[ \hat{F} = \sigma \left[ \frac{\rho \kappa \hat{n}}{\frac{1}{2} \left( \Sigma \rho_{q} \right)} \right] \]  

(4 - 6)

\[ n = \nabla \cdot \alpha_{q} \]  

(4 - 7)

\[ \hat{n} = \frac{n}{|n|} \]  

(4 - 8)

\[ \kappa = \nabla \cdot \hat{n} \]  

(4 - 9)

In addition to the VOF model, we also employ a wall-adhesion model. This model modifies the surface normal vector of the cells near the wall, based on the contact angle the droplet makes with the wall. This results in a dynamic adjustment of the curvature of the droplet surface at the wall. The modified surface normal vector is

\[ \hat{n} = \hat{n}_{w} \cos(\theta_{w}) + \hat{t}_{w} \sin(\theta_{w}) \]  

(4 - 10)

Where \( \hat{n}_{w} \) and \( \hat{t}_{w} \) are the unit vectors normal and tangential to the wall, respectively, and \( \theta_{w} \) is the user specified wall contact angle. The wall contact model works with the CSF model to determine the local curvature \( \kappa \) at one unit cell away from the wall. This value is then applied to all the wall boundaries.
Chapter 5. Microfluidic Droplet Generation and Interaction

5.1. Introduction
Microfluidics is the branch of fluid study dealing with devices and methods of controlling fluids on length scales on the order of micrometers, or sometimes smaller. It has seen significant study in the last two decades [20]. Flow on the micrometer level encompasses systems with very small sample sizes which enables the fluid samples to be analyzed very quickly and at significantly less cost than previous methods. Operating such systems on such small length scales allow for control of laminar flow, short diffusion distances, and hereto unmatched capacity for control and flow manipulation. Accelerated development of the field has led to the development of functional tools for fluid manipulation, such as mixing devices, pumps, and separators [20]. The dominant focus of microfluidic study has been two-phase flow as it provides crucial insight into successful design for several applications, including heating, mixing, reactions, and the potential for scale up systems.

This chapter will focus on the simulation of droplet generation and dynamics in liquid-liquid flows. Specifically, as the droplets travel through a microfluidic chamber designed as a diverging/converging channel. This simulation will attempt to recreate experimental work in order to obtain a method of modelling droplet-droplet interactions in a multi-phase simulation using the Volume of Fluid method. This kind of channel is often encountered in natural porous matrixes and offers the ability to observe the functionalities of multiphase flows. Droplet generation is controlled via liquid flow rates and droplet-droplet interactions are simulated via a numerical scheme to prevent coalescence.

5.2. Literature Review
Two immiscible fluids coming into contact with one another is the basis for all multiphase flow systems. Gas–liquid[21,22] and liquid–liquid flows [42,24-26] are the most common configurations seen in multiphase flow. These systems of multiphase flow in microfluidic devices span a diverse array of applications including reaction[27], mixing [28,29], emulsions[30], biomedicine[31] and material synthesis[32-35]. In these systems, droplet size, population, flow pattern and behavior all must be precisely understood in order to achieve the desired results or specific end. Microfluidics is uniquely positioned to offer such control due to the small length and flow scales as well as the flexibility in device fabrication. Individual droplets of liquid in another liquid or gaseous bubbles in a liquid are easy to control in experiment and can therefore be used to gain a better understanding of multiphase systems. The mechanisms that control droplet or bubble interaction can be studied in great detail.

There is no shortage of studies done regarding both liquid-liquid and liquid-gas multiphase flow in microfluidic devices. Several resources discuss multiphase flows[36,37] and liquid–liquid flows[38-40] Much work has been done concentrating on multiphase flows, with specific interest in droplet flow and generation[41] We will discuss the fundamentals of two-phase flows, two phase flow regimes, and droplet formation.

5.2.1. Two-Phase Flows - Fundamentals

Two-phase or multiphase flows are much more suited to studying several fundamental fluid phenomena, including interfacial area, transfer distance, mixing, and mass transfer. The properties of any two-phase flow in a microfluidic device, are dependent on the properties of the individual fluids, the nature of the flow itself, and the design and geometry of the channel in which the flow occurs. How these properties manifest themselves as dimensionless parameters tells us what the flow will be like.
One of the most important dimensionless numbers in all of fluid mechanics is the Reynolds number (Re). This number balances the contributions of inertial and viscous forces to the flow,

\[ Re = \frac{\rho UL}{\mu} \]  

(5 – 1)

\( \rho \) is the density of the fluid, \( U \) is the velocity of the fluid, \( \mu \) is the viscosity of the fluid and \( L \) is some characteristic length, usually the channel diameter, or the hydraulic diameter in non-circular channels. In microfluidic systems, Re is usually on the order of 1 or less than 1.

The Bond number (BO) relates the forces of gravity to that of interfacial tension in a multifluid system,

\[ Bo = \frac{\Delta \rho g L^2}{\sigma} \]  

(5 – 2)

Where \( \Delta \rho \) is the density difference between the two phases, \( g \) is the acceleration due to gravity, and in this case the characteristic length is usually the droplet diameter. It is used with the Morton number to characterize the shape of droplets moving in a fluid.

The Morton Number (Mo) is defined as:

\[ Mo = \frac{g \mu_c^4 \Delta \rho}{\rho_c^2 \sigma^3} \]  

(5 – 3)

Where the subscript “c” denotes those properties are the properties of the continuous fluid, not the droplet. The Bond number measures the ratio of gravitational (or buoyancy forces) to the forces of surface tension. In microfluidic systems, Bo and Re are much less than one. In this regime, viscous forces and interfacial forces are paramount. Therefore, the Capillary number (Ca) becomes of critical importance. The Capillary number compares the effects of interfacial tension and viscosity, and is critical to the design and flow of microfluidic devices.
\[ Ca = \frac{\mu U}{\sigma} \]  

(5 - 4)

Where \( \sigma \) is the surface tension. Surface tension causes capillary pressure between the two phases at the phase interface, which results in a curved interface.

Of additional importance are some dimensionless numbers which are themselves combinations of other dimensionless numbers. The Weber number (We) and Ohnesorge number (Oh) are both combinations of the Reynolds and Capillary numbers but arranged in two different ways. The Weber number balances the inertial forced with surface tension and the Ohnesorge number compares viscous forces to that of inertial forces combined with surface tension.

\[ Oh = \left( \frac{Ca}{Re} \right)^{1/2} = \frac{\mu}{(\rho L \sigma)^{1/2}} \]  

(5 - 5)

\[ We = Re \cdot Ca = \frac{\rho U^2 L}{\sigma} \]  

(5 - 6)

The relative importance of either Ca or We number depends on the Reynolds number. For low Reynolds number, the Capillary number is the parameter of interest. For high Reynolds number, the Weber number is the parameter of interest. Surface tension is unimportant if either the Weber or Capillary number is much greater than one.

Additional dimensionless parameters which govern the flow are the ratios of the fluid properties of the continuous and dispersed phase. Specifically, the ratios of density, flow rate, and viscosity.

\[ \alpha = \frac{\rho_c}{\rho_d} \]  

(5 - 7)

\[ \beta = \frac{\mu_c}{\mu_d} \]  

(5 - 8)
\[ \varphi = \frac{Q_c}{Q_d} \quad (5-9) \]

The design of the microfluidic system plays a decisive role in droplet formation, and maintaining similar characteristic channel lengths – and thus similar dimensionless numbers – across a given geometry is essential for flow control and droplet formation.

5.2.2. Interfacial phenomena

In microfluidic systems, interfacial effects become the dominant forces which govern the interactions between two fluid systems. These effects include both the fluid-fluid interface, as well as the fluid-wall interface. How the fluid interacts with the wall in a microfluidic channel, the so called “wetting,” determine the nature of the fluid flow. Whether a surface is so called “water wet” or “oil wet” (hydrophobic or hydrophilic) is expressed quantitatively by contact angles of the droplet formation of the dispersed phase (oil or water, respectively). Contact angles less than 90 degrees will only produce flow patterns that can be described as disordered. If the angle is above 90 degrees, flow patterns can reliably produce droplets.[44].

The ability to control two phase flow in microfluidic devices is well understood. The design of microfluidic devices play a critical role in the control and development of liquid-liquid flows. There are various geometries that can be used in order to manipulate the flow in a two fluid system:

5.2.3. T-junction.
The T-junction is one of the most frequently used geometries in a two fluid system, especially to induce flow between two immiscible fluids.[42] The T-junction can operate in two ways: cross-flowing or perpendicular flowing. In cross flowing, the continuous phase flows horizontally and the dispersed phase is introduced via a channel which is perpendicular to the flow of the continuous fluid. In perpendicular flow, the dispersed phase originates in the perpendicular channel. The perpendicular channel has been shown to produce droplets with a more uniform size as compared to the cross-flow configuration.

Two kinds of flow regimes can be produced in the T-junction: droplet and plug flow. The different regimes are defined by the relative flow rates of the two immiscible phases. In plug flow, the plug length is determined by the ratio of the flow rates of the two fluids, and the total flow rate, if the device has a cross flow configuration as its geometry. However, in perpendicular flow, the plug length is only effected by phi. The dependence on flow rate disappears.[45] In droplet flow, the formation of droplets in either the cross flow or perpendicular flow geometry is the same [46]. While the dispersed phase flow rate does not have any effect on the diameter of the droplet, the droplet diameter and continuous fluid flow rate do have a linear relationship. This relationship also extends to the total flow rate.

At low flow rates, the interfacial forces are the dominant forces of the system, which allow for the sharp droplets. If viscous forces increase, or if the flow increases significantly, the forces of surface tension are not enough to produce a sharp break up. The dispersed phase will flow along the channel for some distance until the plug is eventually sheared off.[47] These regimes have also been reproduced in droplet formation studies involving a T-junction, where they are called the squeezing, dripping and jetting regimes, respectively.[48]
Both the plug and droplet flow regimes are also observed in a perpendicular flow system. For plug flows, there is an observable phenomenon where the pinch point of the dispersed phase forms as the plug crosses the point where the continuous phase enters interface. Once the plugs are pinched off, the continuous phases retreats and the cycle of plug generation begins again, with a new plug forming from the perpendicular channel. A similar model happens in droplet flow, though the neck of the dispersed phase formed in smaller than in plug flow.

5.2.4. Flow focusing.

The next most common configuration is the flow focusing junction, which is widely used for the production of spherical droplets of a relatively uniform size.[49] In this configuration, the continuous phase enters the main channel via two side channels, and contacts the dispersed phase at a focus point. At this focus point, the dispersed phase forms a droplet, which flows into the continuous phase down the channel. The flow focusing junction will more often generate droplets rather than plugs due to the geometry of the constriction point where the channels meet, however, it is possible to develop plug flow under certain flow conditions.

There are two regimes that result from the flow focusing junction, called dripping and jetting, corresponding to low flow rates and high flow rates, respectively.[50]. Highly spherical droplets are characteristic of the dripping regime. As the flow increases, and the system approaches the jetting phase, a neck of dispersed phase forms in the channel, and the droplets shear off further downstream, away from the junction point.

Flow control in a flow focusing junction can be achieved by controlling either the flow rate of the two phases, or the inlet pressure of the two phases.[51] The droplet size is directly
related to flow rate, and increases linearly with flow rate. If pressure inlet is controlled, there are two points of critical pressure which exist. At the first, droplet formation occurs and the size of the droplets is consistent. Above the second critical pressure level, droplet size increases rapidly with increased pressure.

5.2.5. Effect of phase parameters

The fluid parameters of each phase in a two fluid system have a dramatic effect on how the system develops droplets. In a microfluidic system, the effects of viscosity and interfacial tension are larger than at macro length scales. The relationship between droplet size and viscosity is a function of the geometry of the channel. Droplet size dependence on viscosity can vary from one type of geometry to another.

At the microfluidic scale, the effects of interfacial tension become prominent, and in some cases, depending on other fluid properties and flow conditions, can be the dominant force governing the interactions between the two fluids. It is customary to require the addition of surfactant in order to achieve the desired interactive properties which favor droplet formation of the dispersed phase. Surfactants in T-junction microdevices have been shown to decrease the droplet diameter, by altering the interfacial forces between the two phases.[42] Droplets with decreased size can also be formed in systems which use flow-focusing junctions as opposed to T junctions or other device configurations.[52]

5.2.6. Coalescence control

The formation of and coalescence of droplets are essential processes whose mechanism of action must be well understood in order to design a device to be used for two-phase flow. Droplet coalescence is useful in several different chemical or physical application such as the mixing of two different reactants for the onset of a reaction, or the mixing of two different
liquid phases carried within a potential third carrier phase. Droplet coalescence is a complex and rapid physical process which occurs over different time and length scales. The mechanics of droplet coalescence can be described in four main stages: approach, drainage of the continuous film, interface breaking, and confluence. Putting our focus towards confluence allows us to be able to accurately predict and model the phenomenon of coalescence between a pair of droplets at the individual droplet level. There are two main methods for facilitating the coalescence of droplets: passive methods, which are designed into the channel geometry itself in order to cause droplets to coalesce, and active methods, which require the use of forces external to the droplet and flow to cause coalescence. Additionally there is an emerging space where control of interfacial rheology of the droplet is used to control coalescence.

5.2.7. Mechanism of two-phase liquid-liquid flows

There has been extensive research on microfluidic multiphase flow, however, despite stable conditions and flow regimes for such devices, total control of the multiphase system necessitates deep knowledge of the mechanisms of droplet generation. There are several approaches that one can take to analyze the physics of droplet flow and formation. The most physically appropriate way is to examine the forces which govern the formation process. These forces are dependent only on a few system variables, and are characterized by the structure and geometry of the microfluidic device as well as the material properties of the channel (and whether that channel is hydrophilic or hydrophobic) and of course the properties of the fluids involved and how those fluids interact with each other. These parameters are weighed against each other as the various dimensionless numbers which govern fluid flow. Because of the scales
involved for microfluidic devices, the most important dimensionless number is the Capillary number (Ca).

There are three typical flow regimes identified in microfluidic channels: dripping, squeezing,[24] and jetting[53]. Correspondingly the T-Junction allows for two different models of the breakup of droplets: shear driven and flow controlled. At Capillary numbers below 0.01 interfacial tension dominates the system, and the phenomenon of the breakup of droplets is controlled by the gradient of pressure within the bubble itself. This is the “rate-of-flow-controlled” mechanism and is seen in virtually all T-junction and flow-focusing geometries. The pressure differential, which drives the breakup, results from the blocking of the channel. Here the droplet size is a function of the flow ratio:

\[
\frac{L}{w} = \varepsilon + \delta \frac{Q_d}{Q_c}
\]

(5 - 10)

where L is the slug length, w is the channel width, Q_d and Q_c are the flow rates, and \(\varepsilon\) and \(\delta\) are empirical values which depend on the geometry.

Different channel geometries require different fitting parameters based on the Capillary number. For low capillary numbers, \((8 \times 10^{-5} < Ca < 8 \times 10^{-3})\) a linear relationship has been observed:

\[
\frac{L}{w} = 1 + \delta \frac{Q_d}{Q_c}
\]

(5 - 11)

Several different fitting parameters have also been proposed[28]

\[
\frac{L}{w} = 1.9 + 1.46 \frac{Q_d}{Q_c}
\]

(5 - 12)
\[
\frac{L}{w} = 1.38 + 2.52 \frac{Q_d}{Q_c}
\]  
(5 – 13)

Above a critical value for the Capillary number, \((Ca < 0.01)\) shear stress plays an important role in the droplet formation process via the mechanism called shear-driven breakup. In such a regime the droplet diameter is inversely proportional to the Capillary number. The droplet diameter \((d_d)\) is then described by

\[
d_d \propto \frac{1}{Ca}
\]  
(5 – 14)

Additionally, droplet diameter is also inversely proportional to continuous phase flow rate and velocity, as well as the total flow rate.

The full mechanism of droplet breakup can be described as follows [54]:

\[
\frac{L}{w} = \varepsilon + k \left( \frac{Q_d}{Q_c} \right)^a \left( \frac{1}{Ca} \right)^b
\]  
(5 – 15)

5.3. Droplet Generation

In order to investigate droplet behavior better, we first have to observe the relationship between flowrate, surface tension, and droplet diameter.

5.3.1. System Setup

A flow focusing droplet generation array is designed with rectangular inlet channels measuring 40 \(\mu m\) by 34 \(\mu m\) for the straight through inlet carrying and 40 \(\mu m\) by 20 \(\mu m\) for the two flow focusing inlets. The entire channel length spans 1 mm. A 3-D model of the system can be seen in Figure 5.1.
Figure 5.1. System Geometry

The boundary conditions for the system are velocity inlets which vary by the specific case being studied and the system has a pressure outlet condition. All the walls are given the no slip condition. The geometry was created in ANSYS design modeler and meshed using the ANSYS meshing tool. The meshing condition was a sweep method where the entire geometry was meshed as individual cubic cells, each with a cell length of 2.5 μm.

Water was chosen as the dispersed phase and oil chosen as the continuous phase, where the dispersed phase enters through the straight through conduit and the dispersed phase enters though flow focusing channels. The fluid properties are given in Table 5.1.

Table 5.1. Fluid properties for simulations comparing flowrate and surface tension to droplet diameter

<table>
<thead>
<tr>
<th>Fluid</th>
<th>$\rho$ (kg/m$^3$)</th>
<th>$\mu$ (cP)</th>
<th>$\sigma_{12}$ (mN/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>998.2</td>
<td>1.003</td>
<td>4.8</td>
</tr>
<tr>
<td>Oil</td>
<td>1614</td>
<td>7.7</td>
<td></td>
</tr>
</tbody>
</table>
5.3.2. Flowrate vs Droplet Diameter

In the first series of cases we examine the influence that flowrate has on droplet diameter. In all cases we modify the continuous fluid flow rate, which in turn determines the total volume fraction of dispersed phase in the system. Table 5.2 shows the various test cases and the associated dimensionless properties for each case, as well as the average droplet diameter generated by the flow focusing junction.

Table 5.2. Table of values for droplet diameter simulation Cases 1-4

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water flowrate (m/s)</td>
<td>0.018</td>
<td>0.018</td>
<td>0.018</td>
<td>0.0180</td>
</tr>
<tr>
<td>Oil flowrate (m/s)</td>
<td>0.0798</td>
<td>0.0625</td>
<td>0.03125</td>
<td>0.0104</td>
</tr>
<tr>
<td>Water volume fraction</td>
<td>0.28</td>
<td>0.33</td>
<td>0.5</td>
<td>0.75</td>
</tr>
<tr>
<td>Re</td>
<td>0.59</td>
<td>0.52</td>
<td>0.4</td>
<td>0.38</td>
</tr>
<tr>
<td>We</td>
<td>0.047</td>
<td>0.032</td>
<td>0.01</td>
<td>0.005</td>
</tr>
<tr>
<td>Ca</td>
<td>0.079</td>
<td>0.062</td>
<td>0.033</td>
<td>0.013</td>
</tr>
<tr>
<td>Observed droplet Diameter (μm)</td>
<td>30</td>
<td>36</td>
<td>42</td>
<td>60*</td>
</tr>
</tbody>
</table>

As expected, we see increasing droplet diameter as the flow rate decreases, and the volume fraction of water increases. One interesting note is that while Case 4 will generate droplets of size 60 μm, the configuration is not stable. Small perturbations will cause the flow focusing mechanism to break and the dispersed fluid will stream straight through the junction without forming droplets. Obviously this result also depends on the particular surface interactions between these two fluids, and a fluid pair with a different surface tension may not yield the same results for these flow conditions. This tells us that there is a critical capillary number below which the flow focusing junction is not stable, and will collapse.
Figure 5.2. Case 1 flowrate vs droplet diameter

Figure 5.3. Case 2 flowrate vs droplet diameter.

Figure 5.4. Case 3 flowrate vs droplet diameter
5.3.3. Surface tension vs droplet diameter

We also examine the case where the surface tension between the continuous and dispersed phase are modified in order to see its effect on droplet diameter. We consider five different cases, keeping the flowrates constant but altering the surface tension between the fluids. The results are reported in Table 5.3.
Here we see that the flow rates and therefore volume fraction does not vary across the simulations, and yet, as in the case with changing flow rate, we reach a point where the dispersed phase does not form droplets at all, but rather continues as a stream unimpeded to the outlet. These tests show us how the droplet formation is governed by the relationship to the capillary number. In both cases an inverse relationship between the capillary number and the effective droplet diameter can be observed. This is consistent with what we observe generally in experimental situations. Because the capillary number is also dependent on viscosity and flowrate, these findings can be translated to microfluidic systems with similar dimensionless properties. The larger unknown is how the geometry of the structure effects the flow, if a flow focusing junction with square channels as opposed to rectangular channels would give the same flow patterns and droplet diameters under the otherwise same conditions. Given that the area of the face of the channel through which the liquid passes directly affects the velocity of the fluid

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water flowrate (m/s)</td>
<td>0.018</td>
<td>0.018</td>
<td>0.018</td>
<td>0.018</td>
<td>0.018</td>
</tr>
<tr>
<td>Oil flowrate (m/s)</td>
<td>0.0798</td>
<td>0.0798</td>
<td>0.0798</td>
<td>0.0798</td>
<td>0.0798</td>
</tr>
<tr>
<td>Water Volume Fraction</td>
<td>0.28</td>
<td>0.28</td>
<td>0.28</td>
<td>0.28</td>
<td>0.28</td>
</tr>
<tr>
<td>Surface Tension (N/m)</td>
<td>0.0048</td>
<td>0.00432</td>
<td>0.00384</td>
<td>0.00528</td>
<td>0.00576</td>
</tr>
<tr>
<td>Re</td>
<td>0.059</td>
<td>0.059</td>
<td>0.059</td>
<td>0.059</td>
<td>0.059</td>
</tr>
<tr>
<td>Bo</td>
<td>0.006166</td>
<td>0.006852</td>
<td>0.007709</td>
<td>0.005606</td>
<td>0.005139</td>
</tr>
<tr>
<td>We</td>
<td>0.047</td>
<td>0.052</td>
<td>0.059</td>
<td>0.042</td>
<td>0.039</td>
</tr>
<tr>
<td>Ca</td>
<td>0.079</td>
<td>0.088</td>
<td>0.099</td>
<td>0.072</td>
<td>0.066</td>
</tr>
<tr>
<td>Droplet diameter (μm)</td>
<td>30</td>
<td>28</td>
<td>-</td>
<td>34</td>
<td>36</td>
</tr>
</tbody>
</table>

Table 5.3. Surface tension vs droplet diameter case study
(in the case of keeping the mass flow rate constant) this would also indirectly effect the capillary number and must be taken into account.

Figure 5.7. Case 1 - Surface tension vs droplet diameter simulation

Figure 5.8. Case 2 - Surface tension vs droplet diameter simulation
Figure 5.9. Case 3 - Surface tension vs droplet diameter - no droplets

Figure 5.10. Case 4 - Surface tension vs droplet diameter simulation
5.4. Three Phase System Test

While the numerical phase change mechanism allowed droplet-droplet interaction, it the nature of the interaction needed to be captured in order to make sure that non-coalescing droplets could successfully be modeled and studied. Therefore a simple simulation was designed to observe the interactions of the droplets of the same material, but with different numerical phase within an enclosed microfluidic device.

We develop a geometry of two intersecting square pipes, with each face having a square inlet with sides of 50 μm. The total length of each section of the pipe from inlet to outlet is 1100 μm. An image of the system geometry can be seen in Figure 5.6.
As before, the three-dimensional geometries were generated in ANSYS Design Modeler and the computational grids were meshed using ANSYS Meshing tool. The inlet channels were truncated to lower the computational resources necessary, but were calculated to be long enough to allow fully developed laminar flow prior to the junction.

The meshing was done using a simple sweep method where every grid cell is a cube of the same size, with side length of 2.5 μm. A full 3-D image of the geometry can be seen in Figure 5.13.
The fluid being introduced via the straight through path in each pipe is the PDMS while the droplets being generated are the water-glycol mixture described earlier. Important to note is that the dispersed phase being introduced at both inlets in the system are coded as different numerical phases in the simulation. While these two dispersed phases have identical physical properties, the system treats them as immiscible separate phases with an interface between them. This will allow us to observe the behavior of two immiscible droplets of the same physical properties that come into contact in a confined space. While in the bulk simulation these droplets will contact in an open area, the confined pipe was chosen in order to minimize computational load when generating the droplets and to ensure collision, as collision in an open environment would not be guaranteed.

Here in Figures 5.14 to 5.17 we can see what happens in the moments before and after droplet collision.
Droplet generation in the system proceeds in a uniform fashion as expected. As the droplets begin to converge in the junction, it appears at first glance as if they coalesce into one large droplet. However, as the simulation progresses, each droplet separately makes its way to the outlet of the system, with their separate interfaces intact. At first glance it appears as though both droplets seem to overlap each other and proceed straight through the junction, but if we isolate each phase separately, we can observe that the surface tension between the droplets causes each of them to make a right turn and exit the system via the other’s outlet stream.

Figure 5.14. Simulation moments before droplet collision
Figure 5.15. Simulation during droplet collision

Figure 5.16. Simulation near the end of droplet collision
In order to determine each droplet phase’s behavior, we look at individual phases one at a time as they progress through the simulation. At the moment of droplet interaction, we can see that the droplets do not cross over one another, but rather squeeze by one another, coalescence inhibited due to the phases having different numerical designations despite being physically identical. This scheme mimics a situation with a strong surfactant and surface tension which prevents coalescence. It will allow for robust droplet-droplet interaction in a regime with lower Reynolds number where the inertial forces are not powerful enough to overcome the forces of surface tension and cause coalescence.
Figure 5.18. Numerical phase 2 of the water-glycol mixture at the moment of droplet interaction

Figure 5.19. Numerical phase 3 of the water-glycol mixture at the moment of droplet interaction
5.5. Numerical Model

5.5.1. Numerical Solution

The commercial software ANSYS Fluent 17 was used to solve the equations and implement a User-Defined Function. Equation coupling was achieved via the PISO (Pressure-Implicit with the Splitting of Operators) method. Pressure interpolation was calculated via PRESTO!, and gradient calculations were done via Green-Gauss node. The momentum equations were calculated via a second-order upwind difference method.

The inlets were all velocity boundaries, and the outlet was a pressure boundary. No-slip conditions were set with a constant contact angle. The variable time stepping method was used to compute the transient simulation, such that the maximum Courant number \( Cr = \Delta t \left( \sum_{i=1}^{n} \frac{u_i}{\Delta x_i} \right) \) during the simulation was 0.25. These simulations were carried out on 20 processors using the SMIC cluster at the High-Performance Computing Facility at Louisiana State University.

The fluid properties used were taken from the experiments done Jose [55], PDMS as the continuous fluid and a water-glycerol mixture consisting of 80% glycerol by volume as the continuous fluid. The density and viscosity of the water-glycerol mixture was calculated based on a volume averaging of the densities of the two liquids. The values of the fluid properties of density, viscosity and surface tension can be seen in Table 5.4.

Table 5.4. Fluid properties used in the simulation

<table>
<thead>
<tr>
<th>Fluid</th>
<th>( \rho ) (kg/m(^3))</th>
<th>( \mu ) (cP)</th>
<th>( \sigma_{12} ) (mN/m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L1</td>
<td>WG80</td>
<td>1208.4</td>
<td>36</td>
</tr>
<tr>
<td>L2</td>
<td>PDMS</td>
<td>965</td>
<td>19</td>
</tr>
</tbody>
</table>
5.5.2. Geometry and Mesh

The system geometry is that detailed in Jose [55] and consists of four chambers: a flow focusing section of square microchannels used to generate monodispersed droplets, a long square microchannel, a diamond-shaped diverging chamber, and a short outlet channel. The continuous fluid (L2) is introduced into both right angle channels with total flow rate $Q_2$ while the dispersed fluid (L1) is introduced in the straight through channel with flow rate $Q_1$. The droplets pinch off at the focusing section and continue on down the long channel towards the diverging chamber. A diagram of the geometry can be seen in Figure 5.20.

![Diagram of microfluidic chamber](image)

Figure 5.20. Diagram of microfluidic chamber
The three-dimensional geometries were generated in ANSYS Design Modeler and the computational grids were meshed using ANSYS Meshing tool. The inlet channels were truncated to lower the computational resources necessary, but were calculated to be long enough to allow fully developed laminar flow prior to the junction. An outline of the full 3-D geometry can be seen in Figure 5.21.

The geometry was meshed using the Assembly Meshing Technique in ANSYS Meshing Tool, and was broken into several different sections with different element grid length in order to decrease the number of elements and increase computation efficiency. The geometry was broken into several sections, each with its own computational element grid length, as can be seen in Figure 5.22. For these simulations, the smallest computational element grid length was used for the sections of the geometry where multiphase flow was likely to occur, with mesh coarseness increasing away from the straight through channel. The unit length used to mesh each section can be found in Table 5.5.
Table 5.5. Lengths of various section of the geometry mesh in Figure 3

<table>
<thead>
<tr>
<th>Section</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>G</th>
<th>H</th>
<th>I</th>
<th>J</th>
<th>K</th>
<th>L</th>
<th>M</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length (μm)</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>10</td>
<td>20</td>
<td>40</td>
<td>40</td>
<td>5</td>
<td>10</td>
<td>20</td>
<td>40</td>
<td>40</td>
<td></td>
</tr>
</tbody>
</table>

Figure 5.22. Sections of the simulation geometry indicating the by single element grid length of the mesh used on that section

5.5.3. Phase Change Mechanism

Under the normal Volume-of-fluid method, any droplet-droplet interaction results in the coalescence of droplets. This is because if any two droplet interfaces of the same numerical phase come into contact within a single computational cell, the system removes the interface and
merges the droplets. This makes modelling droplet-droplet interactions of the same numeric phase impossible in standard VOF. In order to implement the phase change mechanism to allow for droplet-droplet interaction, a User-Defined-Function (UDF) was written and implemented over a specific volume in the geometry downstream of the junction but upstream of the open chamber. Three volumes were defined within the function, corresponding to volumes in the geometry, called an “entrance region,” a “phase change region,” and an “exit region.” These volumes are all continuous, with a single plane separating the entrance region from the phase change region and another plane separating the phase change region from the exit region. The full code of the UDF can be found in Appendix B

![Diagram of the area of the simulation geometry with emphasis on the region defined to implement the Phase Change Mechanism UDF](image)

Figure 5.23. Outline of the simulation geometry with emphasis on the region defined to implement the Phase Change Mechanism UDF

The location of the intersecting planes are defined along the appropriate axis such that the entrance and exit regions are very small, approximately one or two grid cells, while the phase change region is large enough to encompass a single droplet. A diagram of the area of the
geometry where the phase change takes place can be seen in Figure 5.23.

In order to properly implement the UDF, we must implement a series of numerical phases whose physical properties are identical to the dispersed phase. In this implementation there are $n$ phases defined, where phase 1 is the continuous phase, and phases 2 through $n$ are the dispersed phases. However, these different dispersed phases do not represent different fluids, but different numerical identifiers for the same fluid. All of these dispersed phases represent the same physical fluid, therefore it is necessary that all the dispersed phases have all the same physical properties, the only difference between them is their numeric identifier. A counting variable $m$ is identified in the UDF and set with minimum value 3 and maximum value $n$. At each time step, the function scans the entrance region, phase change region, and exit region for the presence of dispersed phase 2 and checks if the concentration is above or below a certain critical value, $\alpha_{2\text{crit}}$. If the concentration of phase 2 is above the critical value in the phase change region, but below the critical value in the entrance and exit regions, this indicates that a droplet has fully entered the phase change region in the geometry. If these conditions are met, the UDF will increase the numeric phase of the dispersed phase in the phase change region. Then the system will move to the next time step and now the droplet, with numeric phase 3, will proceed through the channel with the same physical and system properties it had when it entered the region. Then the counter is increased by 1. The sequence then begins again with a droplet of dispersed phase 2 entering the chamber, and being converted into dispersed phase 4, and so on. This ensures that if contact is made between this droplet and another in the channel, coalescence will not occur. A solution flow diagram of the UDF can be seen in Figure 5.24.
5.6. Results and Discussion

The use of the VOF method for modeling droplet formation was validated by testing various droplet lengths and periods produced in the simulation with the experimental data reported in Jose [55]. In these experiments they define the droplet length as the distance from the leading edge of one droplet to its trailing edge, and they define the droplet distance as the...
The distance between the trailing edge of one droplet to the leading edge of the next droplet in the channel.

The experiments used various fluid pairs to develop relationships between droplet formation and various system properties. In all cases the continuous fluid was PDMS with differing viscosity and the dispersed fluid was some mixture of water and glycerol with different volume percent mixture.

5.6.1. Mesh Dependence

A mesh dependence study was conducted on the droplet formation channel using three different meshes. The edge lengths of the individual grid elements were 2 μm, 5 μm, and 10 μm respectively. The flow rates for the were \( Q_1 = 100 \ \mu\text{L/min} \), and \( Q_2 = 400 \ \mu\text{L/min} \).

The average droplet diameter and droplet spacing are compared in Table 5.6. Since the variations for the fine and medium grids were less than 5%, the medium grid was chosen for the flow focusing junction as well as the portion of the chamber where straight line droplet transit occurs. This is depicted in Figure 5.3 and Table 5.2. The lengths of the channels were determined to be long enough to generate fully developed laminar flow prior to the flow focusing junction.

Table 5.6. Comparison of the droplet length and droplet spacing found in experiment[23] and the various grid resolutions used to determine mesh dependence

<table>
<thead>
<tr>
<th>Droplet Formation</th>
<th>Experiment</th>
<th>Simulation - Grid Resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Coarse</td>
</tr>
<tr>
<td>Droplet Length, ( d_0 ) (μm)</td>
<td>249</td>
<td>230</td>
</tr>
<tr>
<td>Droplet Spacing ( L_0 ) (μm)</td>
<td>308</td>
<td>400</td>
</tr>
</tbody>
</table>
5.6.2. Droplet formation

Adjusting the flowrates at the boundaries for the system allows control of both the droplet length, $d_0$, as well as droplet spacing, $L_0$. The controlling parameters are the flow rate ratio $\varphi$, and the droplet concentration (or, volume fraction) $\alpha_1$.

\[
\varphi = \frac{Q_1}{Q_2}
\]

\[
\alpha_1 = \frac{Q_1}{(Q_1 + Q_2)}
\]  \hspace{1cm} (5 - 16)  \hspace{1cm} (5 - 17)

We will focus on dilute systems ($\alpha_1 \leq 0.5$) as it allows us to produce a consistent droplet size (where the droplet size is approximately the same as the channel height), however there can be a large variance in droplet spacing. Looking at the experimental work of Jose [55], we compare the droplet formation of systems with different volumetric flow rates. These combinations can be seen in Table 5.7. We are attempting to observe the droplet properties and how they are affected by flowrate in the inlet microchannel before they reach the open chamber. Consistent with the work of Jose [55], we measure normalized droplet size $d_0/h$ as a function of $\alpha_2 Ca_2$ (where $Ca_2$ is the Capillary Number with respect to fluid 2, and is defined by $Ca_2 = \frac{\eta_2 Q_2/(\sigma_{12} h^2)}{\eta_2 Q_2/(\sigma_{12} h^2)}$) and observe the same relationship seen in experiment, $d_0/h = 0.5(\alpha_2 Ca_2)^{-0.17}$. This can be seen in Figure 5.24.

Table 5.7. Flowrates used for the simulations studying droplet formation

<table>
<thead>
<tr>
<th>Simulation</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q₁ (μL/min)</td>
<td>4</td>
<td>10</td>
<td>20</td>
<td>30</td>
<td>40</td>
<td>50</td>
<td>60</td>
<td>70</td>
<td>80</td>
<td>90</td>
<td>100</td>
</tr>
<tr>
<td>Q₂ (μL/min)</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>400</td>
<td>400</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>0.01</td>
<td>0.025</td>
<td>0.05</td>
<td>0.075</td>
<td>0.1</td>
<td>0.125</td>
<td>0.15</td>
<td>0.175</td>
<td>0.2</td>
<td>0.225</td>
<td>0.25</td>
</tr>
</tbody>
</table>
Figure 5.25. Results of the simulations regarding droplet formation in the microchannel. Circles represent data taken from simulation while squares represent data taken from Jose[23].

The droplet velocity in the straight channel, $V_0$ is measured via the videos compiled from the images of individual time steps in the simulation. This is compared with the superficial velocity $J_0 = (Q_1 + Q_2)/h^2$ as a function of the Capillary number (here defined as $Ca = \eta_2 J_0/\sigma_1$) in the channel. As in experiment, we see the droplet velocity exceed the superficial velocity and correspond to curve $V_0/J_0 = 1 + 2.5Ca^{2/3}$. This is most evident just after the flow focusing junction where there is noticeable acceleration of the droplet into the channel.

In the dilute regime (on which we are focused) the droplet spacing $L_0$, can be controlled as a function of the previously defined flow ratio, $\varphi$. While it is true that droplet size is dependent on both volume fraction and Capillary Number, the droplet spacing in dilute regimes is independent of absolute flow velocity and then data of the simulation again correspond to experiment where $L_0/d_0 = 0.45\varphi^{-1}$.
5.6.3. Steady State Influence on open chamber dynamics

In order to study the influence of the potentially evolving continuous fluid flow, simulations were performed in order to determine if the system had reached steady state prior to the introduction of the first droplet. For this a flow rate of $Q_2 = 400 \, \mu\text{L/min}$ was chosen and $Q_1$ was set to zero. A solution for the steady state system was calculated with these flow rates, and the resulting flow pattern displayed in Figure 5.27.

A transient simulation was then performed with the same flow conditions in order to calculate the time to reach steady state. The time step was set to $t = 10^{-6} \, \text{seconds}$. Steady state was considered achieved when the values of the solutions to the continuity and momentum equations remain unchanged with a residual of $10^{-4}$. We see the evolution of the steady state
system at several time steps in Figure 5.28.

![Streamline diagrams showing the evolution of the simulation from rest to a steady state solution](image)

Figure 5.27. Streamline diagram showing the evolution of the simulation from rest to a steady state solution where \( Q_2 = 400 \mu L/min \) was chosen and \( Q_1 = 0 \). a) is the system at \( t=0.0001 \) s. b) \( t=0.001 \) s. c) \( t=0.01 \) s. d) \( t=0.02 \) s. The time it takes to reach steady state is 0.018 seconds. Therefore, it is not expected for the droplet trajectory to be effected by the evolution of the continuous fluid towards steady state. Simulations were run where the initial conditions correspond to the continuous fluid at rest and the continuous fluid already at steady state. This is to investigate the degree to which the initial conditions of the continuous fluid have an effect of the trajectory of the dispersed droplet at various flow rates. The show that the initial conditions of the continuous fluid do not greatly impact droplet trajectory.
5.6.4. Droplet distance and single droplet array

We also examined the distance between consecutive droplets in the simulation to determine how they compare to experiment. This distance is an important factor which governs flow assembly and higher ordering structures. In single droplet arrays, the trajectory of the droplets follows a straight line through the chamber, with an observable deceleration as the divergent channel is entered and an observable acceleration as the channel begins to converge. The distance between two consecutive droplets, \( L \), for a given time \( t \), was measured from the rear position of the first droplet \((x_r)\) to the front position of the second droplet \((x_f)\), where \( L(t) = x_r(t) - x_f(t) \). Three different simulations were performed where \( Q_2 = 400 \, \mu\text{L/min} \), and \( Q_1 \) was set to three different flowrates: 2 \( \mu\text{L/min} \), 4 \( \mu\text{L/min} \), and 10 \( \mu\text{L/min} \) respectively. In the first two instances, \( L \) was large enough between any two droplets that the droplets never made contact during the entire run. However, for \( Q_1 = 10 \, \mu\text{L/min} \) the droplets did come into contact with one another as they passed through the channel. This is in contrast to experiment, where the droplets did not contact each other even at this flowrate. The droplet-droplet interaction was not significant enough to cause divergence in the droplet trajectory, but did cause an increased acceleration of droplets to the exit channel. The simulation where \( Q_1 = 10 \, \mu\text{L/min} \) was also performed on a geometry with the fine mesh to determine if the droplet-droplet interactions were a function of too coarse a mesh, however the results remained the same. Due to the droplet-droplet interactions, the UDF was implemented in these simulations in order to prevent artificial coalescence. The number of artificial dispersed phases was set to 2, so there were 3 phases total. Images of the droplet spacing in the chamber as well as a comparison of simulation to experimental results can be seen in Figures 5.29 and 5.30. We can see that the simulation closely replicates the experimental
results for the droplet spacing and trajectory for the given flowrates, with the exception of droplet contact for the highest flowrate.

Figure 5.28. Single droplet propagation arrangement in simulations where \( Q_2 = 400 \, \mu\text{L/min} \) and a) \( Q_1 = 2 \, \mu\text{L/min} \), b) \( Q_1 = 4 \, \mu\text{L/min} \), and c) \( Q_1 = 10 \, \mu\text{L/min} \)
Figure 5.29. Droplet spacing $L$ normalized by initial spacing $L_0$ as a function of dimensionless distance $x/h$. Solid lines are simulation and dashed lines are data taken from Jose[23] for flow rates $Q_2=400 \, \mu$L/min and $Q_1=2, 4, \text{and } 10 \, \mu$L/min

5.7. Conclusions

This chapter presents a simulation of multiphase droplet generation in a converging/diverging microchannel. A User-Defined Function is implemented in order to allow the VOF-model to prevent coalescence of droplets of the same numerical phase. The droplet formation process is compared with experiment and found to closely match results obtained elsewhere. Droplet size was easy to control and predictable. Similarly, the droplet progression along the channel mimics that of experiment, and the UDF successfully allows for droplet-droplet interaction in the channel without coalescence occurring. Since the phase-change volume of the geometry is confined to a small area, the UDF and additional phase does not add a significant computational cost to the VOF-model. This model could be expanded to higher phase numbers, but at greater potential computational cost.
Chapter 6. Summary

In conclusion, we summarize the contributions of this work.

6.1. Subcooled Boiling Multiphase Flow

A Euler-Euler simulation of two phase flow has been used to model subcooled boiling in a pipe with constant heat flux. These results were compared to and validated against experiment. Bubble diameter and nucleation site density are the best predictors of vapor fraction. While several variables were found to be in good agreement with experiment, the model used to calculate bubble diameter across the radius of the system was not as predictive. A population balance model was able to give results which better predicted the shape of the curve of variables of interest, with adjustments necessary to achieve more reliable results.

6.2. Liquid-Liquid Droplet Generation and Interaction

A simulation of multiphase droplet generation in a converging/diverging microchannel was developed. A User-Defined Function was implemented in order to allow the VOF-model to prevent coalescence of droplets of the same numerical phase. The droplet formation process is compared with experiment and found to closely match results obtained elsewhere. Similarly, the droplet progression along the channel mimics that of experiment, and the UDF successfully allows for droplet-droplet interaction in the channel without coalescence occurring. Since the phase-change volume of the geometry is confined to a small area, the UDF and additional phase does not add a significant computational cost to the VOF-model. This model is predictive of droplet-droplet interaction in microfluidic systems at low Reynolds number.
Appendix A. Equations and constants used in turbulence modeling, Chapter 2

The values of the constants with the subscript “3” are determined using a blending function such that for any given constant $\Phi$,

$$\Phi_3 = F_1 \Phi_1 + (1 - F_1) \Phi_2$$  \hfill (A - 1)

$$\nu_t = \frac{a_1 k}{\max(a_1 \omega, SF_2)}$$  \hfill (A - 2)

$$\nu_t = \frac{\mu_t}{\rho}$$  \hfill (A - 3)

$$P_k = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \frac{\partial U_i}{\partial x_j} - 2 \frac{\partial U_k}{\partial x_k} \left( 3 \mu_t \frac{\partial U_k}{\partial x_k} + \rho k \right)$$  \hfill (A - 4)

$$P_{kb} = -\frac{\mu_t}{\rho} g_i \frac{\partial \rho}{\partial x_i} \hfill (A - 5)$$

$$P_{\omega b} = \frac{\omega}{k} \left( (a_1 + 1) \max(P_{kb}, 0) - P_{kb} \right)$$  \hfill (A - 6)

$$F_1 = \tanh(\arg_1^4) \hfill (A - 7)$$

$$\arg_1 = \min \left( \max \left( \frac{\sqrt{k}}{\beta' \omega' \gamma}, \frac{500 \nu}{\gamma^2 \omega}, \frac{4 \rho k}{C_{D_{kw} \sigma_{\omega 2} \omega^2 \gamma^2}} \right) \right) \hfill (A - 8)$$

$$C_{D_{kw}} = \max \left( \frac{2 \rho}{\sigma_{\omega 2} \omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i}, 10^{-10} \right) \hfill (A - 9)$$
Appendix B. Bubble coalescence and breakup models, Chapter 3

The Lou and Svendsend Breakup Model:

\[ g(m_i; f_{BV}m_i) = 0.923F_B(1 - r_d) \left( \frac{m_i}{d_i^2} \right)^{1/3} \int_{\xi_{min}}^{1} \frac{(1 + \xi)^2}{\xi^{11/3}} e^{-\chi} d\xi \]  \hspace{1cm} (B - 1)

\[ \chi = \frac{12\left(f_{BV}^{2/3} + (1 - f_{BV})^{2/3} - 1\right)\sigma}{\beta \rho_c \varepsilon_c^{2/3} d_i^{5/3} \xi^{11/3}} \] \hspace{1cm} (B - 2)

\[ \xi_{min} = \frac{ER_{min} \eta}{d_i} \] \hspace{1cm} (B - 3)

\[ \eta = \left(\frac{1}{\varepsilon_c}\right)^{1/4} \] \hspace{1cm} (B - 4)

Where \( \xi \) is the dimensionless size of eddies in the inertial subrange of isotropic turbulence.

\( ER_{min} \) is the minimum eddy ratio. \( F_B \) is a calibration coefficient, \( \beta = 2 \), \( \varepsilon_c \) is the continuous phase eddy dissipation rate, \( \nu_c \) is the continuous phase kinematic viscosity, and \( \sigma \) is the surface tension coefficient.

The Prince and Blanch Coalesce Model is as follows:

\[ Q(m_i; m_j) = (\Theta^T_{ij} + \Theta^B_{ij}) \eta_{ij} \] \hspace{1cm} (B - 6)

\[ \eta_{ij} = e^{-t_{ij}/\tau_{ij}} \] \hspace{1cm} (B - 7)

\[ t_{ij} = \left(\frac{\rho_c r_{ij}^3}{16\sigma}\right)^{1/2} \ln\left(\frac{h_0}{h_f}\right) \] \hspace{1cm} (B - 8)

\[ \tau_{ij} = \frac{r_{ij}^{2/3}}{\varepsilon_c^{1/3}} \] \hspace{1cm} (B - 9)
\[r_{ij} = \left(\frac{1}{2} \left(\frac{1}{r_i} + \frac{1}{r_j}\right)\right)^{-1}\]  

\[\Theta_{ij}^F = F_{CR} S_{ij} (u_{ti}^2 + u_{tj}^2)^{1/2}\]  

\[S_{ij} = \frac{\pi}{4} (d_i + d_j)^2\]  

\[u_{ti} = \sqrt{2} e_c^{1/3} d_i^{1/3}\]  

\[\Theta_{ij}^B = F_{CB} S_{ij} |U_{rj} - U_{ri}|\]  

\[U_{ri} = \sqrt{\frac{2.14 \sigma}{\rho_c d_i} + 0.505 g d_i}\]
Appendix C. C-Code used for numerical phase change in droplet-droplet interaction, Used in Chapter 5

#include "userdefinedfunction.h"
#include "meshmetric.h"

/****************************************************************************
*/
static int mesh_component=0; /*choose mesh component for entrance/exit criteria
(0=x,1=y,2=z) */
static real entrance_min=0.00064,entrance_max=0.00065;
static real exit_min=0.00076,exit_max=0.00077;
static real zero_vof_tol = 0.001; /* don't reduce below .1 % */
static int phase_counter=1; /* you don't have to change this, is the phase_index for first secondary_phase */
    /* may have to use C_UDMI() for this in the future */
static int num_dispersed_phases=3; /* total number of dispersed phases */
static int zone_ID =2;
static const int init_dis_phase_index=1; /* =1 for first secondary phase */
/****************************************************************************
*/
static real entrance_init_phase_vof_sum=0,entrance_vol_sum=0,exit_init_phase_vof_sum=0,exit_vol_sum =0, mid_init_phase_vof_sum=0,mid_vol_sum=0;
static real exit_new_phase_vof_sum=0,mid_new_phase_vof_sum=0,exit_new_phase_vof_avg=0,mid_new_phase_vof_avg=0;
static real entrance_init_phase_vof_avg=0,exit_init_phase_vof_avg=0,mid_init_phase_vof_avg=0;
static real phase_counter_incrementing=1; /* Toggle to turn-off incrementation when only continuous phase is present */
/****************************************************************************
*/
DEFINE_ADJUST(change_disp_phase,d)
{
    Domain *domainstate;
}
domaistaten = Get_Domain(1);

Threadlookup *tm;
tm = Lookup_Thread(domain,zone_ID);

Thread *t_init_dis_phase;
Thread *t_new_dis_phase;

Thread *ft;
Thread **pt;

cell_t c;
face_t f;

real x[ND_ND];

int new_dis_phase_index;

entrance_init_phase_vof_sum = 0, entrance_vol_sum = 0, exit_init_phase_vof_sum = 0, exit_vol_sum = 0,
mid_init_phase_vof_sum = 0, mid_vol_sum = 0; /* RESET gloabl variables */
exit_new_phase_vof_sum = 0, mid_new_phase_vof_sum = 0, exit_new_phase_vof_avg = 0, mid_new_phase_vof_avg = 0; /* RESET gloabl variables */
entrance_init_phase_vof_avg = 0, exit_init_phase_vof_avg = 0, mid_init_phase_vof_avg = 0; /* RESET gloabl variables */

new_dis_phase_index = init_dis_phase_index + phase_counter;

#if !RP_HOST
begin_c_loop_int(c,tm)
{
/* For Avg vof of init_dis_phase in entrance-section */
C_CENTROIDMESH(x,c,tm)
((x[mesh_component] > entrance_min) & (x[mesh_component] < entrance_max))
{
entrance_init_phase_vof_sum += C_VOF(c,t_init_dis_phase)*C_VOLUME(c,tm);
entrance_vol_sum += C_VOLUME(c,tm);
}
/* For Avg vof of init_dis_phase in exit-section */
if((x[mesh_component] > exit_min) & (x[mesh_component] < exit_max))
{
exit_init_phase_vof_sum += C_VOF(c,t_init_dis_phase)*C_VOLUME(c,tm);
exit_vol_sum += C_VOLUME(c,tm);
}
/* For Avg vof of init_dis_phase in mid-section */
if((x[mesh_component] > entrance_min)&&(x[mesh_component] < exit_min))
{
    mid_init_phase_vof_sum += C_VOF(c,t_init_dis_phase)*C_VOLUME(c,tm);
    mid_vol_sum += C_VOLUME(c,tm);
    /* Message0("mid_init_phase_vof_sum = %g \n",mid_init_phase_vof_sum);
        Message0("mid_vol_sum = %g \n",mid_vol_sum); */
}

/* For Avg vof of new_dis_phase in exit-section */
if((x[mesh_component] > exit_min)&&(x[mesh_component] < exit_max))
{
    exit_new_phase_vof_sum += C_VOF(c,t_new_dis_phase)*C_VOLUME(c,tm);
}

/* For Avg vof of new_dis_phase in mid-section */

C_CENTROID(x,c,tm)
if((x[mesh_component] > entrance_min)&&(x[mesh_component] < exit_min))
{
    mid_new_phase_vof_sum += C_VOF(c,t_new_dis_phase)*C_VOLUME(c,tm);
}

/* Message("Before sync In Node %d   ,mid_init_phase_vof_sum is : %g \n",myid,mid_init_phase_vof_sum); */

/* NODE synchronization */
PRF_GSYNC();
entrance_init_phase_vof_sum = PRF_GRSUM1(entrance_init_phase_vof_sum);
exit_init_phase_vof_sum = PRF_GRSUM1(exit_init_phase_vof_sum);
mid_init_phase_vof_sum = PRF_GRSUM1(mid_init_phase_vof_sum);

entrance_vol_sum = PRF_GRSUM1(entrance_vol_sum);
exit_vol_sum = PRF_GRSUM1(exit_vol_sum);
mid_vol_sum = PRF_GRSUM1(mid_vol_sum);

exit_new_phase_vof_sum = PRF_GRSUM1(exit_new_phase_vof_sum);
mid_new_phase_vof_sum = PRF_GRSUM1(mid_new_phase_vof_sum);

/* Message("After sync In Node %d   ,mid_init_phase_vof_sum is : %g \n",myid,mid_init_phase_vof_sum); */
node_to_host_real_1(entrance_init_phase_vof_sum);
node_to_host_real_1(exit_init_phase_vof_sum);
node_to_host_real_1(mid_init_phase_vof_sum);
node_to_host_real_1(entrance_vol_sum);
node_to_host_real_1(exit_vol_sum);
node_to_host_real_1(mid_vol_sum);
node_to_host_real_1(entrance_vol_sum);
node_to_host_real_1(mid_vol_sum);
node_to_host_real_1(mid_vol_sum);
node_to_host_real_1(exit_new_phase_vof_sum);
node_to_host_real_1(mid_new_phase_vof_sum);

#if RP_NODE
    /* Compute mean vof in the 3 sections */
    entrance_init_phase_vof_avg = entrance_init_phase_vof_sum/entrance_vol_sum;
    exit_init_phase_vof_avg = exit_init_phase_vof_sum/exit_vol_sum;
    mid_init_phase_vof_avg = mid_init_phase_vof_sum/mid_vol_sum;
    exit_new_phase_vof_avg = exit_new_phase_vof_sum/exit_vol_sum;
    mid_new_phase_vof_avg = mid_new_phase_vof_sum/mid_vol_sum;
    /* Message("In Node %d ,mid_init_phase_vof_avg is : %g\n",myid,mid_init_phase_vof_avg); */
    node_to_host_real_1(entrance_init_phase_vof_avg);
    node_to_host_real_1(exit_init_phase_vof_avg);
    node_to_host_real_1(mid_init_phase_vof_avg);
    /* Message0("In Node %d ,entrance_init_phase_vof_avg is : %g\n",myid,entrance_init_phase_vof_avg);
    Message0("In Node %d ,exit_init_phase_vof_avg is : %g\n",myid,exit_init_phase_vof_avg);
    Message0("In Node %d ,mid_init_phase_vof_avg is : %g\n",myid,mid_init_phase_vof_avg);
    Message0("In Node %d ,mid_init_phase_vof_avg is : %g\n",myid,mid_init_phase_vof_avg);
    */
    Message0("phase_counter = %d\n",phase_counter);
    Message0("new_dis_phase_index = %d\n",new_dis_phase_index);
    Message0("phase_counter_incrementing = %d\n",phase_counter_incrementing);
#endif
if
((entrance_init_phase_vof_avg<zero_vof_tol)&&(exit_init_phase_vof_avg<zero_vof_tol)\&\&mid_init_phase_vof_avg>zero_vof_tol)
{
    phase_counter_incrementing = 1;
    Message0("_If condition is true \n",myid);

    begin_c_loop_int(c,tm)
    {
        C_CENTROID(x,c,tm)
        if((x[mesh_component]> entrance_max)\&\&(x[mesh_component]< exit_min))
        {
            C_VOF(c,t_new_dis_phase)=C_VOF(c,t_init_dis_phase)+C_VOF(c,t_new_dis_phase);
            /* C_VOF(c,t_new_dis_phase)=C_VOF(c,t_init_dis_phase); */
            C_VOF(c,t_init_dis_phase)=0;
        }
    }end_c_loop_int(c,tm)

    mp_thread_loop_f(ft,d,pt)
    {
        begin_f_loop_int(f,ft)
        {
            F_FLUX(f,pt[new_dis_phase_index])=F_FLUX(f,pt[init_dis_phase_index])+F_FLUX(f,pt[new_dis_phase_index]);
            F_FLUX(f,pt[init_dis_phase_index])=0;
        }
    }end_f_loop_int(f,ft)

    /*
    begin_f_loop_int(f,tm)
    {
        F_CENTROID(x,f,tm);
        if((x[mesh_component]> entrance_max)\&\&(x[mesh_component]< exit_min))
        {
            F_FLUX(f,t_new_dis_phase)=F_FLUX(f,t_init_dis_phase)+F_FLUX(f,t_new_dis_phase);
            F_FLUX(f,t_new_dis_phase)=0;
        }
    }end_f_loop_int(f,tm)
    */
}

else  /* check if the phase_changed drop has moved out, then update counter */
{
    Message0("_Else condition is true \n",myid);

}
if ((exit_new_phase_vof_avg < zero_vof_tol) && (mid_new_phase_vof_avg < zero_vof_tol) && (phase_counter_incrementing == 1))
{
    phase_counter+=1; /* increment phase_counter as soon as the drop leaves, ... */
    phase_counter_incrementing =0; /* ... but not in the subsequent iterations */

    Message0("__If_2 condition is true \n",myid);
}
if(init_dis_phase_index+phase_counter==num_dispersed_phases)
{
    phase_counter=1; /* reset phase_counter */
    Message0("__If_3 condition is true \n",myid);
}
#endif /* !RP_HOST */
} /* End of DEFINE_ADJUST*/
References


88


90


Vita

Aaron Harrington was born in 1985 in Miami, Florida, USA to Kurt and Dena Harrington. He completed his Bachelor’s degree in Chemical Engineering at the University of Florida in 2008. After spending some time in the private sector he decided to pursue an advanced degree in Chemical Engineering at Louisiana State University in the Fall of 2012. During his studies, in June 2017 he welcomed the birth of his daughter, Giselle.

Aaron is a movie and trivia buff who likes to spend his free time listening to audiobooks, and enjoys all things tech. He plans to receive his Masters Degree in December 2021.