NUMERICAL SIMULATION OF CRYOGENIC FLOW WITH PHASE CHANGE USING SHARP INTERFACE CUT-CELL METHOD

By

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To my mother
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Cryogenic fluids find wide use in many different types of industries as well as space applications, where they may be used as the liquid fuel or the cryogen for other vital support systems. Therefore the transportation, handling and storage of cryogenic flow under microgravity in space missions is an important design concern. During their transportation through the pipes in a spacecraft, because of strong heat flux from wall, a rapid quenching process with voracious boiling of the cryogen takes place. This can subject the piping system to extreme thermal stresses due to sudden contraction. Due to strong vaporization and resulting two-phase flow, the mass flow rate of cryogenic flow will decrease. The insufficient flow rate can cause many problems in the spacecraft. Therefore a thorough physical understanding of the phase change phenomenon in cryogenic flow under microgravity is very important. Investigation of cryogenic chill down under microgravity is not easy because it is not easy to create the microgravity conditions on earth. Most of the experiments on quenching under microgravity have been done on board special aircrafts like NASA’s KC-135. The cost of performing these experiments is very high. Moreover, it is not easy to collect experimental data in flight.

In this research work, numerical simulation techniques are used instead of experiments. In numerical simulation, the microgravity is easily modeled and the cost is much less than performing experiments. The sharp interface method (SIM) with cut-cell technique (SIMCC) is adopted to handle the two-phase flow computations. In SIM, the background
grid is the Cartesian grid and the explicit interfaces are embedded in the computation domain dividing the entire domain into different sub-domains corresponding to various phases. In SIM, each phase has its own set of governing equations. The interfacial conditions act as the link between different phases. The cut-cell technique is utilized to handle the non-rectangular cells produced by the intersection of interfaces with the Cartesian grid. The conservative properties of the finite volume method can be satisfied better near the interface using cut-cells. The interface is treated as an entity with zero thickness with no volume association. With the explicit geometrical information about the interface and high resolution numerical schemes, the heat flux near the interface can be evaluated more accurately than by any other multiphase techniques.

This research aims to expand the scope of the SIMCC method by several enhancements like multigrid methods and third-order upwind differencing scheme for the convective term. These enhance the performance and stability of the SIMCC and improve its capability to handle the very challenging task of simulating internal multiphase flows. The specific focus of this research is inverted annular film boiling regime. Various physical mechanisms that influence the flow patterns and heat transfer characteristics during the transportation under reduced gravity are investigated.
CHAPTER 1
INTRODUCTION

1.1 Overview

Cryogenic fluids find wide use in many areas, ranging from space propellants, space life support systems, cryogenic hardening of metals to increase hardness and durability, cooling superconducting magnets such as those used in MRI and NMR, cryo-preservation of blood and biological materials, cryosurgery, and other chilling and freezing applications. Common cryogenic fluids are liquid nitrogen, hydrogen, helium, oxygen and argon among others. In space explorations, gases like hydrogen and oxygen are often stored in liquid form due to their high ratio of weight to volume leading to efficient storage. They are used for power launching of space vehicles. Therefore, the efficient and safe transport and storage of cryogenic fluids under microgravity are important design considerations in space applications.

1.2 Role of Cryogenics in Space Missions

Cryogenic fluids have many applications in spacecrafts. Liquid hydrogen is used as a fuel provides the advantage of efficient storage and more power per gallon. Liquid oxygen is used as an oxidizer for hydrogen or other fuels. Liquid methane also finds potential use as propellant in space applications [1]. In space explorations, there is a huge incentive for improving the technology for the storage and transport of cryogenic fluids. For example, the ability to use hydrogen as fuel means that a given mission can be accomplished with a smaller quantity of propellants (and a smaller vehicle), or alternately, that the mission can be accomplished with a larger payload than is possible with the same mass of conventional propellants. The efficient and safe utilization of cryogenic fluids in thermal management, power and propulsion, and life support systems of a spacecraft during space missions involves the transport, handling, and storage of these fluids in reduced gravity conditions. The uncertainties about the flow pattern and heat transfer characteristics pose difficulties for design of equipment.
1.3 Cryogenic Chill Down Process

When any cryogenic system is started up, including rocket thrusters, turbo engines, reciprocating engines, pumps, valves, and pipelines, it must go through a transient chill down period prior to a steady state operation. Chill down is the process of introducing the cryogenic liquid into the system, and allowing the hardware to cool down to several hundred degrees below the ambient temperature. This large temperature drop occurs very rapidly. As reported by researchers [2–4] it may be complete in 20-30 seconds. Therefore it requires highly skilled technical knowledge to chill down a cryogenic system in a safe and efficient manner.

The highly unsteady chill down process is extremely complex because when a cryogenic liquid is introduced into a system which is at ambient temperature, voracious evaporation occurs and a very high velocity vapor mist traverses through the system. As the system cools, slugs of liquid, entrained in the vapor, flow through the system in a two-phase film boiling mode. As the system cools further, a liquid quenching front flows through the system and is accompanied by nucleate boiling and two-phase flow. The rate of heat transfer in the nucleate boiling regime is very high and the system begins to cool down very rapidly. As the system rapidly cools down, the two-phase flow passes through several flow regime transitions to single-phase liquid flow. The inherent danger during chill down is that two-phase flows are inherently unstable and can experience extreme flow and pressure fluctuations. The hardware may be subject to extreme thermal stresses due to thermal contraction and may not be able to sustain extreme pressure fluctuations from the cryogen.

Efficiency of the chill down process is also an important issue since the cryogen used to chill down the system can no longer be used for propulsion or power generation. To economize, the chill down must be accomplished with a minimum consumption of cryogen in order for the overall energy efficiency to be within tolerable limits. In order for liquid hydrogen to be adopted as the fuel of choice, it is important to fully understand the
thermal-fluid dynamics associated with the chill down process and develop predictive models that reliably predict the flow patterns, pressure loss, heat transfer rates, and temperature history of the system.

1.4 State of the Art

In general, there is very little heat transfer data for cryogenic flow boiling in reduced gravity. The main reason is that both experimental and numerical studies into the phenomenon pose severe challenges. For performing experiments on the transient quenching process, microgravity conditions need to be produced. Drop towers and parabolic flight aircrafts like NASA’s KC-135 aircraft are required. Therefore these experiments are expensive and difficult to perform. On the numerical side, the complexities of the two-phase flow patterns make it difficult to simulate the phenomenon directly. Use of two-fluid models has been made to study some of its aspects [5, 6]. [7] attempted a direct numerical simulation of the cryogenic chill down process with a limited scope.

The present research focuses on addressing specific fundamental and engineering issues related to the microgravity two-phase flow and boiling heat transfer of cryogenic fluids. It provides physical understanding of the transport physics of cryogenic boiling and two-phase flows in reduced gravity by using numerical techniques.

1.5 Objectives of this Research

The scientific objective of this research is to study the fundamental aspects of microgravity cryogenic chill down process for the inverted annular film boiling regime. The simulation will specifically focus on the effect of reduced gravity. This research will further the understanding of the complex interaction of various processed taking place like heat transfer characteristics due to film boiling, surface tension effects, effect of the mass flow rate, to name a few. The engineering objective is to address issues that are related to the design of systems associated with the transport and handling of cryogenic fluids,
for example, pressure drop information through pipes and heat transfer coefficients for inverted annular film boiling.

1.6 Scope and Structure

The goal of the present research is to investigate the transportation of cryogenic flow in microgravity with the phase change phenomena, with focus on inverted annular film boiling flow. It is difficult and expensive to perform experimental research on cryogenic flow because of the limited ways of producing reduced gravity conditions on earth. In this research, the numerical tools will be developed to investigate this interesting area. Therefore the scope of this research will be:

1. To investigate the rate of vaporization (mass loss of cryogenic liquid) based on different driving mechanisms ($Ja, Re$ etc.) and the effect of wall boundary.

2. To calculate the transient film boiling heat transfer coefficient and temperature distributions of wall during the chill down process.

3. To calculate the above for different types of cryogenic fluids, for example liquid nitrogen, oxygen and argon.

4. To develop the necessary numerical techniques for phase change computation in the context of internal flows.

The overall thrust is to develop an accurate and efficient numerical package for simulating the cryogenic flow in microgravity to help in the design of the most reliable cryogenic transportation system in space missions or related industrial applications.

In this dissertation there are eight chapters. In the first two chapters, the literature about heat transfer and phase-change characteristics of cryogenic flow, the impact of microgravity and the flow patterns in the chill down processes is reviewed. In chapter three, the physical model and related governing equations and interfacial conditions are explained. In chapter four, the numerical techniques about the solver of governing equation, moving interface technique, the sharp interface method with cut-cell treatment (SIMCC), phase change computation and the multigrid technique for SIMCC will be introduced. In chapter five, a series of test cases are done to ensure that the current
numerical techniques are accurate and reliable. In chapter six, the results of numerical simulations for cryogenic chill down of Liquid $N_2$, $O_2$ and $Ar$ have been presented. In chapter seven, the results for engineering heat transfer coefficients are analyzed and compared with literature. The last chapter summarizes the current research and presents some ideas for future directions.
CHAPTER 2
LITERATURE REVIEW

2.1 The Boiling Curve and Phase Change Processes

The heterogeneous boiling process occurring at the surface of a body in an extensive pool of essentially quiescent liquid is referred to as pool boiling. Pool boiling can be understood in terms of the so-called boiling curve, as shown in Figure 2-1, which is a plot of the heat flux $q''$ versus the wall superheat $T_w - T_{sat}$ on the logarithmic scale. The liquid is assumed to be at its saturation temperature $T_{sat}$. As the wall superheat increases, the fluid goes through natural convection, formation of isolated bubbles or partial nucleate boiling (A-B), formation of slugs and columns of fully developed nucleate boiling (B-C), transition boiling (C-D) and finally film boiling beyond the point D up to E. The point C on the curve corresponds to the critical heat flux (CHF). This is the case for temperature controlled boiling process. In a boiling process where heat flux is controlled, if the heat flux is increased beyond the CHF, the fluid jumps horizontally from point C to point E and directly enters the film boiling regime without the transition boiling phase. After the CHF is reached, most of the surface is covered with vapor and becomes nearly insulated [8]. This makes the surface temperature rise very rapidly. Therefore the CHF marks the safe limit of operation for many boiling systems.

A chill down or quenching process proceeds in the reverse direction on the boiling curve. It usually starts above point E in the post-CHF region and then goes towards point D in the film boiling regime as the wall temperature decreases. Point D is called the Leidenfrost point which signifies the minimum heater temperature required for the film boiling. For the film boiling process, the wall is so hot that liquid will vaporize before reaching the heater surface that causes the heater to be always in contact with vapor. When cooling beyond the Leidenfrost point, if a constant heat flux heater were used, then the boiling would shift from film to nucleate boiling (some where between points A and B)
directly with a substantial decrease in the wall temperature because the transition boiling is an unstable process.

### 2.2 Convective Boiling in Tubes and Channels

Convective boiling, i.e. boiling that takes place in the presence of forced convection in tubes and channels, offers a very rich variety in terms of observed flow patterns due to the interaction of the forced convection, gravitational effects and the boiling process. The observed flow type depends on several factors like the mass flow rate, the void fraction, the orientation of pipe, the fluid properties and the heat flux at the wall of pipe [9].

Figure 2-2 is an example that shows the different two-phase flow types in a horizontal pipe. The flow types may be bubbly flow, plug flow, stratified flow, wavy flow, slug flow or annular flow [10]. Figure 2-2 [11] is another example and shows the flow regimes of a two phase flow in a vertical tube with upward flow direction. In this case, the possible flow types are bubbly flow, slug flow, churn flow, annular flow and mist flow. The main difference between the horizontal and vertical flows is the effect of gravity that causes the horizontal flow to become non-symmetrical to the tube centerline.
The vertical quenching of a pipe in terrestrial gravity has received a lot of attention due to its importance in the Loss Of Coolant Accident (LOCA) safety considerations in the nuclear power industry. [12] studied in great detail the the flow regimes and heat transfer characteristics in a vertical pipe quenching. They found that for steady injection rate of coolant, the observed flow pattern depended on whether the liquid was subcooled.
or not, as shown in Figure 2-4. For the case of subcooled liquid, an inverted annular film boiling (IAFB) regime is observed above the liquid column. This is not the case for a saturated liquid, where the flow regimes show an annular film boiling type pattern above the region of nucleate boiling. In both the cases, above the inverted annular or annular flow region, dispersed flow film boiling (DFFB) regime was observed. DFFB is characterized by varying size drops and globs of fluid dispersed in the vapor phase. The heat transfer mechanism is film boiling. As the wall temperature reduces to a certain degree, the liquid phase is able to contact the tube wall somewhere upstream of the film boiling region. The leading liquid-wall contact point, which is often referred to as the quenching front (QF) or sputtering region, is characterized by voracious boiling with large decrease in the wall temperature. The quenching front propagates downstream with the flow. The heat transfer mechanism at the QF is transition boiling and the flow is very agitated in this region. This re-establishment of liquid-wall contact is called rewetting phenomenon and has been a research topic for several decades. Thus, studies of quenching in terrestrial gravity (1-g) show that the flow patterns existing are quite different from those observed under adiabatic or even boiling but non-quenching conditions.

The flow patterns also depend on the flooding rate at QF and the inlet water velocity [13–15]. If the inlet mass flow rate is low, then the vapor quality at the QF is high which results in annular film boiling regime. Conversely, if the inlet mass flow rate is high, then the vapor quality at the QF is low and IAFB exists. There have been relatively few studies about these quenching flow patterns which occur at very high heat fluxes (greater than CHF) and the heat transfer mechanisms are not as well understood. A good paper discussing the hydrodynamic aspects of post-CHF flows is [16]. [13] have reviewed some of the heat transfer aspects and correlation work for DFFB. IAFB in terrestrial gravity has been studied using two-fluid models [17, 18], homogeneous flow models [19, 20] and separated flow models [10].
Figure 2-4. Flow patterns during quenching of a supported hot tube

2.3 Two-Phase Flow in Microgravity: Experiments

Most of the experiments on boiling in microgravity ($\mu$-g) have been aimed at understanding the basic mechanisms of pool boiling, bubble generation and boiling incipience, by changing the level of gravity [21–23]. Two-phase flow under adiabatic conditions in microgravity has also been studied for some time. [24–26] have focused on the two-phase flow regimes, void fraction and pressure drop under steady state conditions. The general understanding from these experiments is that in $\mu$-g the distributed flow regimes such as bubbly and dispersed flow occur over a wider range of qualities than under normal gravity (1-g).

However, these experiments on steady-state flow or pool boiling are not very useful for understanding quenching processes in microgravity, as even in terrestrial gravity quenching flow patterns are quite different from adiabatic or even boiling flows [27]. Quenching experiments conducted under $\mu$-g show that there are certain similarities and differences in the flow characteristics which would be important in the design of thermal components for space applications. Most of these experiments have been performed on board NASA’s KC-135 aircraft [2–4, 28]. Two types of data were obtained from these experiments- a set
of large number of visual recordings of the quenching process inside a quartz tube, and the thermal characteristics established during the injection of the coolant into a stainless steel tube. Table 2-1 summarises some of the experiments on quenching in microgravity performed by various researchers.

Table 2-1. Microgravity quenching experiments

<table>
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<th>Observed Flow Pattern</th>
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<td>[28]</td>
<td>14mm ID, 1.2m long quartz tube with Freon (R-113) at atmospheric pressure</td>
<td>IAFB, DFFB</td>
</tr>
<tr>
<td>[3, 29]</td>
<td>1.05 cm ID, 1.274 cm OD, 60 cm long quartz tube and 0.432 cm ID, 0.635 cm OD, 70 cm long SS tube with Liquid $N_2$</td>
<td>Filamentary flow</td>
</tr>
<tr>
<td>[30]</td>
<td>SS flat surface, using a micro heat flux and surface temperature sensor with Freon (R-113)</td>
<td>IAFB</td>
</tr>
<tr>
<td>[31]</td>
<td>6 mm ID pyrex tube with transparent 100 nm Indium-Tin Oxide coating for heating, FC-72 liquid</td>
<td>IAFB and bubbly flow</td>
</tr>
</tbody>
</table>

2.3.1 Two-Phase Flow Patterns in Microgravity

It is essential to have an accurate knowledge about the flow patterns existing under quenching conditions before any attempt at modeling the phenomenon can be made. Although the quenching process is quite complex, but in microgravity the orientation of the pipe should not make any difference to the observed two-phase flow pattern or heat transfer characteristics. There would be no stratification in the flows in microgravity.

In cryogenic chill down experiments, there may be a difference of several hundred degrees between the initial cryogen and tube wall temperatures. When the coolant enters the hot tube, the wall temperature is much higher than the Leidenfrost point, and the liquid evaporates very quickly forming a vapor film, which does not allow the liquid
to contact the wall of the tube, thus leading to inverted annular film boiling (IAFB). The flow patterns observed in \( \mu \)-g during the series of quenching experiments with a transparent quartz tube [28] and R-113 were predominantly inverted annular flow and dispersed droplet flow regimes. The inverted annular-like flow regime in \( \mu \)-g showed a much thicker vapor film as compared to 1-g conditions. They observed a thick liquid filament flowing freely through the thick vapor layer. The filament was not axisymmetric, due to small fluctuations in the g-level. There was much less bubble entrainment due to high subcooling of the liquid. The liquid core was often much thinner, resembling a liquid filament rather than the typical IAFB under terrestrial gravity. ‘It was smooth and continuous, and flowed mostly in the middle of the tube, sometimes almost filling up the whole volume’ [28]. In the entire duration of their tests, rewetting of the wall by the liquid did not take place.

Another important experiment was performed by [29]. They used liquid \( N_2 \) in their experiments, which was injected at varying pressures to control the coolant flow rate and at different wall temperatures into a quartz tube. They initially observed only vapor, followed for a short period by dispersed flow, which was then replaced by what they call as “filamentary” flow. The liquid took the form of long liquid filaments surrounded by a vapor blanket separating them from the tube wall. They were able to observe quenching in their experiments, during which the flow pattern was not very clear. The passage of the QF was followed by nucleate boiling region and fully liquid regime.

In another experiment [3] report that the surface of the filament appeared to be highly turbulent. The liquid seemed to be confined to these filaments, with no appreciable droplets or liquid masses. The filamentary flow was observed in nearly all of the low gravity cryogenic chill down tests, and occurred for all the coolant flow rates they tested.

In a recent study by [31] with FC-72 liquid, it was found that the mass flow rate of the liquid had a significant effect on the stability of the liquid core in IAFB, both under terrestrial gravity and microgravity. Figure 2-5 shows the observed flow patterns.
in their study for microgravity. For low mass flow rates and 1-g, the inverted annular flow was observed but the interface was characterized by high level and disorder and was very unstable. At higher mass flow rates, the IAFB was much more stable. In \( \mu \)-g, the liquid core was much more stable than in 1-g, with the higher mass flow rate case being more stable. The stability of the liquid core is attributed to the small difference relative-velocities of the liquid and vapor phase for the higher mass flow rates. As discussed in [10], the primary mechanisms of interface instability are the Rayleigh-Taylor and Kelvin-Helmholtz instabilities. Therefore it is to be expected that in the absence of gravity and for lower relative velocity of the two phases, the liquid core will be more stable.

### 2.3.2 Heat Transfer in Microgravity

In general, there is little heat transfer data for cryogenic flow boiling in reduced gravity. [30] have investigated the flow film boiling during quenching of R-113 on a hot
flat surface. They used microsensors to record instantaneous heat flux and heater surface temperature during the film boiling on board a KC-135 aircraft. They reported lower heat transfer rates during microgravity as compared to normal gravity and contributed that to thickening of the vapor layer. The wall superheat and the surface heat flux at the onset of rewetting and maximum heat flux were found to increase with the inlet liquid subcooling, mass flux and gravity level. The effect of gravity was determined to be more important for low flow rates and less relevant for high flow rates.

[3] have reported that the quench process is delayed in low gravity and the tube wall cooling rate was diminished under microgravity conditions. The absence of Rayleigh-Taylor instability in microgravity enhances the stability of the interface, contributing to the lowering of the rewetting temperature. [4] have reported a drastic decrease in the film boiling heat transfer rates during the quenching of a tube under microgravity.

2.4 Two-Phase Flow in Microgravity: Numerical Models

In this research, the main objective is to simulate the cryogenic chill down process under reduced gravity such as encountered in space to obtain the design parameters for the related equipment. The most important factor is the absence of gravity. The entire flow field should be controlled by the forced convection, pressure gradient and viscous effects only. Some surface-tension induced forces and wall surface effects will also contribute. When the dynamics is changed, the flow regime will also be changed.

Isothermal two-phase flow in channels or pipes has been well researched. A classical problem is that of an air finger propagating in a viscous liquid in a two-dimensional channel. The velocity of the tip of the air bubble remains constant as it travels in the channel, assumed to be infinite. This is called the Bretherton problem and is used as a benchmark case for two-phase fluid infused type problem in a channel or tube. It has been studied extensively by researchers [32–35].

There have been several attempts to model the cryogenic chill down process under normal gravity. [5] look at stratified flow film boiling in horizontal pipes. They looked at
the circumferential variation in temperature and heat transfer due to the stratification of the two-phase flow. The IAFB and DFFB have also been well researched for normal gravity conditions, as these are important flow regimes which can occur just before the Loss Of Coolant Accident (LOCA). This is because transition boiling and then film boiling takes place when the critical heat flux (CHF) has been exceeded. In film boiling, due to the intervening vapor layer between the liquid core and the tube wall, a burnout of the component is possible. Notable papers on IAFB using the two-fluid model are [17, 18, 36].

Figure 2-6. Comparison between measured and predicted wall temperatures under microgravity with flow rate of 40 cc/s [Reprinted with permission from Yuan K. et al. 2009, Numerical modeling of cryogenic chilldown process in terrestrial gravity and microgravity (Page 51 Figure 5). International Journal of Heat and Fluid Flow, 30]

A recent paper by [6] is one of the first attempts to model cryogenic two-phase flow in reduced gravity. In their model, they have included IAFB and DFFB regions as well as the single-phase liquid with nucleate boiling and pure vapor zones since these are the flow patterns observed in \( \mu \)-g condition by researchers. They use a two-fluid model for IAFB and DFFB. The model results indicate that film boiling heat transfer decreases with decreasing gravity level. They achieved good agreement with experimental results in their model. Figure 2-6 shows their results for the wall temperature as a function of time.
There has been a significant amount of research in the numerical simulation of multiphase flows as well. Until about twenty years ago, these problems were considered too complicated to be solved in entirety, and only analytical solutions for limiting cases [37] were attempted. However, due to an exponential increase in computing power in the recent years, they can now be solved by direct numerical simulation.

In some of the early research done on multiphase flows, many researchers preferred to use curvilinear grids [38–42]. This approach can be used for very simple multiphase flows with only a single embedded object. In order to describe the deformation of the interface powerful grid generation is required. The grid has to be updated frequently to obtain a convergent solution, making it very computationally intensive. In recent years, several Cartesian grid methods have been introduced: the Sharp Interface Method (SIM) [43, 44], the Immersed Boundary Method (IBM) [45, 46], the Volume-of-Fluid (VOF) method [47, 48], the Level-Set method [49, 50], the hybrid Level-Set and Volume-of-Fluid method [51, 52], the Phase-Field method [53] etc. Based on the computational framework, SIM and IBM are classified as mixed Eulerian-Lagrangian while the Level-set, VOF and Phase-Field methods are in the Eulerian category [54]. [55] provides a good review about the respective strengths and advantages of the Sharp Interface Methods (SIM) and the Continuous Interface Methods (CIM) for microgravity applications.

To the best of the author’s knowledge, the only attempt at directly simulating cryogenic flows in microgravity using the full set of equations for fluid flow and heat transfer is by [7] with a limited scope. This work will be referred to time and again in this research, as the basic numerical techniques are the same, with deviations and enhancements which are specific to this research.
CHAPTER 3
PROBLEM STATEMENT AND GOVERNING EQUATIONS

In this chapter, the physical problem to be studied in this research is defined. The model of the complex two-phase flow transitions that take place during cryogenic chill down is based on observation of physical phenomena. As noted in the literature review, for most part of cryogenic chill down process in microgravity the flow is in inverted annular regime, with film boiling at the surface. This is because in cryogenic chill down process, there may be a difference of several hundred degrees between the initial cryogen and tube wall temperatures. Figure 3-1 is a schematic of a cryogenic system, where liquid cryogen is stored in the tank and flows through a pipe to be used in other devices. When the coolant enters the hot tube, the wall temperature is much higher than the Leidenfrost point, and the liquid evaporates very quickly forming a vapor film, which does not allow the liquid to contact the wall of the tube, thus leading to inverted annular film boiling (IAFB). Therefore, it is reasonable to simplify the problem and study only the inverted annular flow. Near the inlet of the tube, a quenching front forms that is followed by an inverted

![Figure 3-1](image_url)

Figure 3-1. Simplified schematic of cryogenic system

annular flow pattern with vapor phase next to the pipe wall and a liquid core in the center [3]. As the liquid vaporizes, the radius of the liquid core would decrease as it travels downstream. Figure 3-2 illustrates the proposed physical model of IAFB in microgravity. In Figure 3-2 the top picture shows real inverted annular flow while the picture in the bottom is that of idealized inverted annular flow with a smooth interface. In the real case, the interface is not smooth due to many reasons like turbulence and instabilities such as the Kevin-Helmholtz instability.
There are several publications about post-CHF flow regimes, i.e., IAFB and DFFB [14, 17, 18, 56–58]. All of them rely on correlations to calculate the heat transfer at the wall and interface. In the present work, no assumption has been made about the temperature or heat flux a priori. The only assumption is that the pipe is insulated from the surroundings. This is reasonable to assume because in many applications it is of interest to minimize the loss of cryogen by evaporation. Therefore in this research the temperature of the wall’s inner surface will vary and so will the heat flux. The heat transfer coefficient will be calculated from the temperature field obtained from the simulations. A conjugate heat transfer model has been used to couple the temperature fields in the wall and the fluid.

The processed occurring inside the tank and other devices downstream of the pipe exit will not be included in the current simulation. Only the straight section of pipe connecting these devices will be considered in this research. In the absence of gravity, it is reasonable to assume the inverted annular flow is axisymmetric. Figure 3-2 shows the model for the idealized continuous inverted annular flow which will be used in the current numerical simulation.
To complete the entire heat transfer path, the two-phase flow inside the pipe must be connected to the heat source, the pipe wall. The wall provides heat by three modes. There are the regular heat conduction and convection mechanisms. Due to the high temperature difference, there will also be radiation from the internal surface of the wall to the liquid core. Figure 3-3 shows the model for conjugate heat transfer of wall and fluid. The external surface of the wall is assumed to be totally insulated. Therefore on the outside of wall the Neumann boundary condition will be assigned.

3.1 Assumptions in the Numerical Model

The basic model consists of single component inverted annular flow in a pipe under microgravity and film boiling. To simplify this model further, the following set of assumptions have been made:

- The geometry as well as the physics of the flow is completely axisymmetric, and 2D cylindrical coordinate system can be used to represent the flow.
- Incompressible flow in both the phases. This assumption is justified because in cryogenic flow, the velocities attained are relatively low \( Ma < 0.3 \). The temperature differences between the two phases are chosen to be moderate in the computations. Due to these factors, the flow can be assumed to be incompressible.
- Constant properties in both the liquid and vapor phases, both of which are Newtonian fluids.
- The flow is laminar, and viscous dissipation can be neglected.
• Thermal equilibrium exists at the vapor-liquid interface, heat transfer in the bulk of fluids and the solid wall.

• The vapor phase is transparent to thermal radiations from the wall, the latter acting as a grey body.

### 3.2 Governing Equations

The Sharp Interface Method with Cut-Cell approach (SIMCC) has been adopted to model the inverted annular two-phase flow problem. SIMCC treats the different phases as discrete, and the interface is treated as a true surface with no volume association. Therefore, if there are $N$ phases, there will be $N$ sets of governing equations, while the transport fluxes at the interfaces are matched by using the appropriate interfacial conditions.

In cryogenic two-phase flow with phase change, the mass, momentum and energy conservations equations are developed separately for the liquid and vapor phase. The interfacial conditions come from the continuity of the tangential velocity and tangential stress, thermal equilibrium between the two phases, and the jump conditions of normal stress and heat fluxes.

#### 3.2.1 Governing Equations for Bulk Phases

The governing equations can be expressed in compact form as follows:

- **Liquid phase:**
  \[
  \mathbf{\nabla} \cdot \mathbf{\bar{u}}_l = 0
  \]
  \[
  \rho_l \left[ \frac{\partial \bar{u}_l}{\partial t} + \mathbf{\nabla} \cdot \left( \mathbf{\bar{u}}_l \mathbf{\bar{u}}_l \right) \right] = -\mathbf{\nabla} p_l + \mu_l \nabla^2 \bar{u}_l
  \]
  \[
  \rho_l C_{pl} \left[ \frac{\partial T_l}{\partial t} + \mathbf{\nabla} \cdot (\bar{u}_l T_l) \right] = k_l \nabla^2 T_l \tag{3-1}
  \]

- **Vapor phase:**
  \[
  \mathbf{\nabla} \cdot \mathbf{\bar{u}}_v = 0
  \]
  \[
  \rho_v \left[ \frac{\partial \bar{u}_v}{\partial t} + \mathbf{\nabla} \cdot \left( \mathbf{\bar{u}}_v \mathbf{\bar{u}}_v \right) \right] = -\mathbf{\nabla} p_v + \mu_v \nabla^2 \bar{u}_v
  \]
  \[
  \rho_v C_{pv} \left[ \frac{\partial T_v}{\partial t} + \mathbf{\nabla} \cdot (\bar{u}_v T_v) \right] = k_v \nabla^2 T_v \tag{3-2}
  \]
• Solid wall:

$$\rho_w C_{pw} \frac{\partial T_w}{\partial t} = k_w \nabla^2 T_w$$  \hspace{1cm} (3-3)

where the subscripts ‘l’, ‘v’ and ‘w’ denote the liquid, vapor and solid phases respectively; $\vec{u}$ is the velocity, $p$ is the pressure, $T$ the temperature, $\rho$ is the density, $\mu$ is the dynamic viscosity, $C_p$ is the specific heat capacity and $k$ is the thermal conductivity.

3.2.2 Interfacial Conditions

The interfacial conditions are derived from continuity, force balance and thermal equilibrium for the interface between the liquid and vapor phase:

• Mass balance:

$$\rho_l (\vec{u}_l - \vec{u}_{int}) \cdot \vec{n} = \rho_v (\vec{u}_v - \vec{u}_{int}) \cdot \vec{n} = \dot{m}''$$  \hspace{1cm} (3-4)

• Force Balance in normal direction:

$$p_l - p_v = \sigma \kappa + \rho_v u_{v,n} (u_{v,n} - u_{int,n}) - \rho_l u_{l,n} (u_{l,n} - u_{int,n}) + \tau_{l,n} - \tau_{v,n}$$  \hspace{1cm} (3-5)

• Energy conservation at the interface:

$$- (k_l \nabla T_l - k_v \nabla T_v - \dot{q}'_{rad}) \cdot \vec{n} = \rho_l \lambda (\vec{u}_l - \vec{u}_{int}) \cdot \vec{n} = \dot{m}'' \lambda$$  \hspace{1cm} (3-6)

• Temperature at the interface:

$$T_l = T_v = T_{int}$$  \hspace{1cm} (3-7)

where the subscript ‘int’ denotes the interface, $\dot{m}''$ is the interfacial mass flux, $\vec{n}$ is the unit normal vector at the interface and $\vec{u}_l$, $\vec{u}_v$ and $\vec{u}_{int}$ are the velocities at the interface of liquid, vapor and interface respectively. $\tau$ denotes the viscous stress, $\sigma$ is the surface tension, $\kappa$ is the curvature and $\lambda$ is the latent heat of vaporization. In this research, radiation effects from the wall will be included for some of the cases. Therefore the term $\dot{q}'_{rad, w}$ denotes the radiative heat flux from the wall incident on the liquid surface:

$$\dot{q}'_{rad} = \sum \left( \frac{T_{w}^{4} - T_{sat}^{4}}{1 - \varepsilon_{w}} \frac{R_{l} \varepsilon_{l}}{R_{wi}} \right)$$  \hspace{1cm} (3-8)

The thermal radiation from the wall surface is:

$$\dot{q}'_{rad, w} = \sum \left( \frac{T_{w}^{4} - T_{sat}^{4}}{1 - \varepsilon_{w}} \frac{R_{w}}{R_{wi}} \right)$$  \hspace{1cm} (3-9)
where $\epsilon_w$ and $\epsilon_l$ are the emissivities of the wall and liquid surface respectively, $R_{wi}$ and $R_l$ are the radii of the surface of the wall and liquid respectively, and $\sigma_S = 5.6697 \times 10^{-8}$ is the Stefan-Boltzmann constant. For the unsteady moving interface problem, these sets of governing equations and interfacial conditions must be satisfied for each time step.

### 3.3 Non-Dimensionalization

In this work all the computational quantities are non-dimensional. The Navier Stokes equation for each phase, the energy equation, as well as the interfacial conditions must be non-dimensionalized first. The reference scales are the diameter $d$ of the pipe, the inlet velocity $U$ and the temperature difference between the wall and boiling point of liquid $T_w - T_{sat}$. The characteristic time is $d/U$. With these reference scales, the dimensionless variables are defined as:

\[ x^* = \frac{x}{d}, \quad u^* = \frac{u}{U}, \quad t^* = \frac{t}{d}, \quad \rho^* = \frac{\rho}{\rho_{ref}}, \quad \mu^* = \frac{\mu}{\mu_{ref}}, \quad T^* = \frac{T - T_{sat}}{T_w - T_{sat}}, \quad k^* = \frac{k}{k_{ref}}, \quad C_{p^*} = \frac{C_p}{C_{p,ref}} \]

Here properties of the liquid phase are used as reference. After the non-dimensionalization procedure, the governing equations and the interfacial conditions can be written as follows (for convenience the asterisks for dimensionless quantities are dropped from this point on):

- **Liquid phase:**
  \[
  \nabla \cdot \vec{u}_l = 0 \\
  \frac{\partial \vec{u}_l}{\partial t} + \nabla \cdot (\vec{u}_l \vec{u}_l) = -\nabla p_l + \frac{1}{Re} \nabla^2 \vec{u}_l \]

- **Vapor phase:**
  \[
  \frac{\partial \vec{u}_v}{\partial t} + \nabla \cdot (\vec{u}_v \vec{u}_v) = -\nabla p_v + \left( \frac{\mu_v}{\mu_l} \right) \frac{1}{Re} \nabla^2 \vec{u}_v \\
  \left( \frac{\rho_v}{\rho_l} \right) \frac{\partial T_v}{\partial t} + \nabla \cdot (\vec{u}_v T_v) = \left( \frac{k_v C_{pl}}{k_l C_{pw}} \right) \frac{1}{Pe} \nabla^2 T_v \]

- **Solid wall:**
  \[
  \left( \frac{\rho_w}{\rho_l} \right) \frac{\partial T_w}{\partial t} = \left( \frac{k_w C_{pl}}{k_l C_{pw}} \right) \frac{1}{Pe} \nabla^2 T_w \]
The interfacial conditions can be expressed in the non-dimensional form in the following way:

- Mass balance:
  \[ \rho_l (\vec{u}_l - \vec{u}_{int}) \cdot \vec{n} = \rho_v (\vec{u}_v - \vec{u}_{int}) \cdot \vec{n} = \dot{m}'' \]  \hspace{1cm} (3-13)

- Force Balance in normal direction:
  \[ p_l - p_v = \frac{\kappa}{We} + \left( \frac{\rho_v}{\rho_l} \right) u_{v,n} (u_{v,n} - u_{int,n}) \]
  \[ - u_{l,n} (u_{l,n} - u_{int,n}) + \frac{1}{Re} \left[ \left( \frac{\partial u_n}{\partial n} \right)_l - \left( \frac{\mu_v}{\mu_l} \right) \left( \frac{\partial u_n}{\partial n} \right) v \right] \]  \hspace{1cm} (3-14)

- Energy conservation at the interface can be rewritten as:
  \[ u_{v,n} - u_{int,n} = \frac{Ja}{Pe} \left( \frac{k_v \partial T_v}{k_l \partial n} - \frac{\partial T_l}{\partial n} + \frac{\dot{q}''}{k_l \Delta T} \right) \]  \hspace{1cm} (3-15)

- Temperature condition:
  \[ T_l = T_v = T_{int} \]  \hspace{1cm} (3-16)

where the dimensionless parameters are:

- Reynolds number: \( Re = \frac{\rho_l U D}{\mu_l} \)
- Peclet number: \( Pe = \frac{\rho_l C_{pl} U D}{k_l} \)
- Weber number: \( We = \frac{\rho_l U^2 d}{\sigma} \)
- Jakob number: \( Ja = \frac{\rho_l C_{pl} (T_w - T_{sat})}{\rho_v \lambda} \)  \hspace{1cm} (3-17)

### 3.4 Computational Domain, Initial and Boundary Conditions

As stated previously, the geometry as well as the physics of the flow is completely axisymmetric, therefore a 2D cylindrical coordinate system can be used to represent the flow. All the governing equations are used in their cylindrical coordinate formulation.

Because of axisymmetry of the pipe, a rectangular domain with a width of 0.5 (non-dimensional pipe radius) is used to simulate the flow field. A graded mesh which is very fine near the interface but coarse away from the interface is used. The minimum grid spacing is 0.01. The initial shape of the liquid annulus is assumed to be a quarter circle,
with a radius 0.38 plus a straight line section with length 0.03. This leaves a gap of 0.12 between the liquid core and the solid wall. This is illustrated in the Figure 3-4. The figure is not to scale.

Figure 3-4. Computational domain for numerical simulation of cryogenic flow through pipe

Initially, the temperature of the wall and vapor inside the pipe is set as $T_w = 1.0$ and $T_v = 1.0$. The cryogen entering the tube is assumed to be at its saturation temperature. Therefore, for the liquid phase, $T_l = 0.0$ is set as the initial condition. At the inlet both the vapor and the liquid are prescribed a unit velocity, whereas the vapor in the flow domain is assumed to be quiescent initially. At the outlet, mass conservation of the vapor phase is enforced. For this purpose, the inlet vapor mass flow and the mass generated at the liquid surface are taken into account. By taking a very long flow domain (for example $L = 44$ for $Re = 3000$), the fully developed boundary condition is ensured at the pipe exit. The top boundary is a wall, therefore we use the no-slip boundary condition for velocity. The bottom boundary is symmetric. The temperature condition needs more attention, since the wall is also included in the computational domain. For the vapor-wall surface, we have

$$T_w = T_v \quad \text{at} \quad r = R_{wi}/D$$

$$k_w \frac{\partial T}{\partial r} = k_v \frac{\partial T}{\partial r} + \frac{\dot{q}_{rad, w} D}{k_l \Delta T} \quad \text{at} \quad r = R_{wi}/D$$

(3–18)
where \( R_{wi} \) is the inner radius of the pipe. \( R_{wo} \) is the outer radius of the pipe. The outer surface of the pipe is assumed to be insulated. Therefore:

\[
\frac{\partial T}{\partial r} = 0 \quad \text{at} \quad r = R_{wo}/D \quad (3-19)
\]
CHAPTER 4
NUMERICAL METHOD FOR MODELLING MULTIPHASE FLOWS

In this section, the numerical method adopted for direct simulation of cryogenic two-phase flow is presented. As explained, a combined Eulerian-Lagrangian framework with the concept of an explicit sharp interface separating the two phases, is central to our approach. In other words, the interface is a true surface without any volume association. The interface is advanced using the normal stress balance. The key elements of the numerical technique are listed below. For more details refer to [7, 59].

4.1 Fractional Step Method for Navier-Stokes Equation

In order to best enforce the conservation laws and to treat the discontinuity at the interface, the finite volume method is used to discretize the governing equations. Within this framework, the governing equations listed before will be integrated over a finite control volume. This is called a unit cell as shown in Figure 4-1. The integral forms of governing equations are given:

Continuity equation:

\[ \int_{cv} (\bar{u} \cdot \bar{n}) \, dV = 0 \]  (4-1)

Momentum equation:

\[ \int_{cv} \frac{\partial \bar{u}}{\partial t} \, dV + \int_{cs} \bar{u} (\bar{u} \cdot \bar{n}) \, dS = - \int_{cs} p\bar{n} \, dS + \frac{1}{Re} \int_{cs} \bar{\nabla} \bar{u} \cdot \bar{n} \, dS \]  (4-2)

where \(cv\) and \(cs\) represent the control volume and the surface of the control volume, respectively. \(\bar{n}\) is the outward normal vector from the control volume surface, \(\bar{u}\) is the velocity vector and \(p\) is the pressure.

A cell-centered collocated (non-staggered) approach [60] on the Cartesian grid system is adopted, the primitive variables (velocity, pressure and temperature) are defined at the cell centers and the primary variables needed at the cell faces are evaluated by interpolation from respective variables at cell centers as shown in Figure 4-1. The
fractional step method is a branch of pressure based predictor-corrector methods. The predict-correct procedure is not determined uniquely and can be constructed by different combinations of prediction and correction procedures. The key point is that the governing equations can not be modified during the prediction procedure and the continuity equation must be included in last correction procedure since the continuity equation is not solved separately. Here, a second order accurate two-step fractional step method \[61–63\] is used for advancing the solutions of the integral unsteady governing equations in time. In this approach, the solution is advanced from time step \(n\) to \(n + 1\) through an intermediate diffusion-convection step. In the intermediate step, the momentum equations without the pressure gradient terms are first solved and advanced. The intermediate diffusion-convection momentum equation can be discretized as:

\[
\int_{cv} \frac{\vec{u}^* - \vec{u}^n}{\Delta t} \, dV = -\frac{1}{2} \int_{cs} \left[ 3\vec{u}^m \left( \vec{U}^n \cdot \vec{n} \right) - \vec{u}^{n-1} \left( \vec{U}^{n-1} \cdot \vec{n} \right) \right] \, dS \\
+ \frac{1}{2 Re} \int_{cs} \left( \vec{\nabla} \vec{u}^* + \vec{\nabla} \vec{u}^n \right) \cdot \vec{n} \, dS \quad (4–3)
\]

where \(\vec{u}^*\) is the intermediate velocity at the cell center and \(\vec{U}\) is the velocity at center of the cell face. The cell surface velocity is used to evaluate the fluxes in or out of a control volume. After \(\vec{u}^*\) is determined, \(\vec{U}^*\), the intermediate velocity at the center of cell face, is calculated by interpolating between the respective cell-center velocities. The first term
on the right hand side is the convective term. A second order accurate Adams-Bashforth scheme is used to discretize the convective term. The second term is the diffusive term that is discretized by the implicit Crank-Nicolson scheme. This eliminates the potential viscous instability that could be quite severe in the simulation of viscous flows. Once the intermediate velocity is obtained, the pressure is obtained by the correction step

\[
\int_{cv} \frac{\vec{u}^{n+1} - \vec{u}^*}{\Delta t} \, dV = - \int_{cv} \vec{\nabla} p^{n+1} \, dV \tag{4-4}
\]

In this pressure correction step, the final velocity \( \vec{u}^{n+1} \) must satisfy the continuity equation in the integral form, which can be written in the following form:

\[
\int_{cs} \left( \vec{U}^{n+1} \cdot \vec{n} \right) \, dS = 0 \tag{4-5}
\]

Therefore, the integral pressure correction equation can be expressed as:

\[
- \int_{cs} \left( \vec{\nabla} p^{n+1} \right) \cdot \vec{n} \, dS = \int_{cs} \left( \vec{U}^* \cdot \vec{n} \right) \, dS \tag{4-6}
\]

Once the pressure is obtained, the intermediate velocity can be corrected and updated to obtain the final velocity by:

\[
\vec{u}^{n+1} = \vec{u}^* - \Delta t \left( \vec{\nabla} p^{n+1} \right)_{cell\,center} \tag{4-7}
\]

\[
\vec{U}^{n+1} = \vec{U}^* - \Delta t \left( \vec{\nabla} p^{n+1} \right)_{cell\,face}
\]

The energy equation is a simple convection-diffusion equation. It is discretized using the finite volume formulation. The diffusion terms are treated with Crank-Nicholson scheme and have second order accuracy with respect to time.

\[
\int_{cv} \frac{T^{n+1} - T^n}{\Delta t} \, dV = - \frac{1}{2} \int_{cs} \left[ 3T^n \left( \vec{U}^n \cdot \vec{n} \right) - T^{n-1} \left( \vec{U}^{n-1} \cdot \vec{n} \right) \right] \, dS \\
+ \frac{1}{2Pe} \int_{cs} \left( \vec{\nabla} T^{n+1} + \vec{\nabla} T^n \right) \cdot \vec{n} \, dS \tag{4-8}
\]

In the energy equation, the non-linear convection terms are treated explicitly. They are discretized using second order Adam’s Bashforth scheme for time, and central differencing
in space. The energy equation is solved using line by line tri-diagonal matrix algorithm (TDMA).

Figure 4-2. An example of cut cells formed near the interface

4.2 Cartesian Grid with Cut-Cells for Treatment of Complex Geometries

In some of the early research done on multiphase flows, researchers preferred to use curvilinear or body-fitted grids [38–42]. This approach can be used for very simple multiphase flows with only a single embedded object. In order to describe the deformation of the interface powerful grid generation is required. The grid has to be updated frequently to obtain a convergent solution, making it very computationally intensive. In recent multiphase computations, several Cartesian grid methods have been introduced: the Sharp Interface Method (SIM) [43, 44], the Immersed Boundary Method (IBM) [45, 46], the Volume-of-Fluid (VOF) method [47, 48], the Level-Set method [49, 50], the hybrid Level-Set and Volume-of-Fluid method [51, 52], the Phase-Field method [53] etc. Based on the computational framework, SIM and IBM are classified as mixed Eulerian-Lagrangian while the Level-set, VOF and Phase-Field methods are in the Eulerian category [54].

In this research, the Sharp Interface Method (SIM) which is type of mixed Eulerian-Lagrangian Cartesian grid method is employed to simulate complex geometries. In SIM, a Cartesian grid forms the background mesh and explicit interfaces are used to describe the shapes of the objects embedded in this background grid. The interface is explicit and is constructed
by a sequence of marker points. With these marker points, the shape and location of the interface are determined by designated interpolation procedures, while the overall fluid flow is computed based on the fixed Cartesian grid. The interfacial dynamics associated with the moving/fixed boundaries is satisfied simultaneously with the bulk fluid flow. The advantage provided by SIM is that it exactly follows the continuum model for fluids. The interface has zero thickness, and there is no approximation involved in either the kinematic or the dynamic model. The primary variables at the interface are computed via the interfacial conditions.

Figure 4-3. Example of mixed structured and unstructured grid

In SIM, one needs to define the relationship between the background grid and the explicit interface. Because the interface does not conform to the grid, the cells containing the interface will be cut and form non-rectangular cut-cells. These cut-cells need to be treated differently from ordinary rectangular cells. In this research, a cut-cell procedure based on [44, 64–66] is employed to treat the cells near the interface. In the cut-cell approach, each segment of the cut-cell is merged into a neighboring cell or assigned the identity of the original Cartesian cell. Hence, even though the underlying grid is Cartesian, the cut cells are reconstructed to become the non-rectangular cells and the cut sides will form the interface. After the reconstruction, the entire grid is filled with the rectangular
structured grid and non-rectangular cells. The shapes of the cut-cells so formed can be triangular, trapezoidal or pentagonal. SIM with the cut-cell approach (SIMCC) can handle the sharp discontinuity in fluid properties resulting from the presence of the interface. Therefore SIMCC can achieve greater accuracy [44, 65]. Among the Eulerian-Lagrangian approaches, SIMCC gives the best accuracy, especially near a solid boundary. Figure 4-3 is an example of the type of grid system used in SIMCC. An explicit interface constructed by marker points will divide the entire domain into different phases. The grid has two types of cells, rectangular cells away from the interface and cut-cells in its vicinity. The cut-cell approach also ensures that the total number of cells does not change during the computation.

4.3 Sharp Interface Method with Cut-cell Technique (SIMCC)

In this research, SIMCC has been adopted to solve multiphase flows with complex geometries. The computational domain consists of regular rectangular cells and the so-called cut-cells. Since the number of cells in SIMCC is not changed during the reorganization of the grid, the matrix of coefficients of SIMCC is very similar to the original one for the cylindrical coordinate system. Only a small percentage of coefficients (those corresponding to the cut-cells) have to be modified so that the convergence behavior and characteristics are very close to that of the curvilinear grid. Therefore it converges much faster than unstructured grid solvers. However, due to the cut-cell algorithms and data management requirements, SIMCC is computationally intensive as compared to diffuse interface methods. Consistent interpolation formulae are chosen for estimation of the fluxes along any of the cell surfaces. Both the convective and viscous terms are calculated using second-order formulae to maintain a globally second-order accurate algorithm. SIMCC can be used to solve fluid flow and heat transfer problems involving more than one phases and/or a complex geometry with a high accuracy.

SIMCC has four main algorithmic procedures: interfacial tracking, the merging procedure, the flux computations in the interfacial region and the moving interface
algorithm for advancing the interface. The first three are needed for a stationary object embedded in the underlying Cartesian grid. Moving interface algorithm is used for advancing the interface for moving or deforming objects and is discussed in the next section.

The cut-cell approach developed in [64] is used to handle irregular intersections between an interface and the Cartesian grid. Because of the interface, some cells are cut and can not maintain their rectangular shape anymore and require special treatment. These cells are called ‘cut-cells’. Figure 4-2 illustrates the formation of cut-cells where the regular grid is cut by the interface.

For interfacial tracking, information about the interface needs to be stored in a way which allows for easy computations. In the present research, positions of marker points are fitted by piecewise-quadratic curves. From these curves, various geometrical quantities like the normal, curvature and the intersections between the interface and background grid can be easily calculated. Information about the intersections is needed to know which cells have been cut by the interface and need to be reconfigured. This information is also used for the next step, the merging procedure.

Using the merging procedure, the fragments of cells intersected by the interface can be merged with neighboring cells or with larger fragments to form the cut-cells. For the purpose of forming cut-cells, the interface is assumed to be formed by a sequence of straight line sections. The possible shapes of cut-cells that can be formed after the merging procedure are trapezoidal, triangular and pentagonal. The new grid is formed by the regular cells and the special cut-cells. Most cells still keep the original shapes. Also, the number of cells does not change.

It is important to know the shape of the newly formed cut-cells for the third technique, which is flux computations. It is also important to know on which side of the cut-cell the interface lies. A special interpolation scheme with a higher order accuracy is required to handle the complicated cut-cells to get the accurate primary variables or
derivatives at a cell face. The interpolation is one-sided in the sense that only the variable values for one phase are used to evaluate the derivatives etc. for that phase.

The original Cartesian grid will now become a mixed grid which includes some structured grid, some of the original grid, and the unstructured grid, the newly generated cut-cells. Figure 4-3 is an example of the mixed structured and unstructured type grid obtained after the merging procedure.

These algorithms and their implementation in the numerical code is explained in the following sections. For more details, please refer to [7, 59].

4.3.1 Interface Representation and Tracking

In SIMCC, the interface is geometrically and kinematically sharp, and represented explicitly by marker points. The location of the marker points is stored, and can be fitted with piecewise continuous and differentiable curves to obtain geometric information about the interface. The Figure 4-3 shows the marker points distributed on the interface.

The location of marker points is stored parametrically as a function of the arc length measured from some reference point on the interface. Since quadratic curves have been used, therefore the functional form of the parametric equations is also quadratic. In fact, all the primary variables are stored in the same format,

$$\phi = a_\phi s^2 + b_\phi s + c_\phi$$

(4–9)

where $\phi$ is the variable to be stored and $s$ is the arc length. The coefficients $a_\phi, b_\phi, c_\phi$ are obtained by the three points that form the piecewise quadratic curve. This enables the calculation of geometric quantities such as the normal and curvature at any given point along the interface:

$$n_x = \frac{-y_s}{(x_s^2 + y_s^2)^{1/2}}$$

$$n_y = \frac{x_s}{(x_s^2 + y_s^2)^{1/2}}$$

(4–10)
Here the subscript $s$ denotes differentiation with respect to the arc length. For the axisymmetric case [66], the curvature $\kappa$ is calculated from

$$\kappa = \frac{x_s}{y (x_s^2 + y_s^2)^{3/2}} + \frac{y_s x_{ss} - y_{ss} x_s}{(x_s^2 + y_s^2)^{3/2}}$$

Once the parametric representation of the interface is obtained and the normal and curvature have been calculated, it is easy to find the intersections between the interface and background grid. Information about the intersections is needed to know which cells have been cut by the interface and need to be reconfigured. This information is also used for the next step, the merging procedure.

### 4.3.2 Cut-Cell Formation and Merging Procedure

Using the merging procedure, the fragments of cells intersected by the interface can be merged with neighboring cells or with larger fragments to form the cut-cells. For the purpose of forming cut-cells, the interface is assumed to be formed by a sequence of straight line sections. The possible shapes of cut-cells that can be formed after the merging procedure are trapezoidal, triangular and pentagonal. The new grid is formed by the regular cells and the special cut-cells.

Figure 4-2 illustrates the formation of interfacial cells where cells 1 to 4 are cut by an interface. According to the present cut-cell technique, the segments of an interfacial cell not containing the original cell center are absorbed by their neighboring cells; the segments containing the original cell center are given the same index as the original cell. For example, in Figure 4-2, the upper segment of cell 3 is absorbed into cell 5 to form a new trapezoid cell. The fraction of cell 3 with cell center becomes a new independent trapezoid cell. The main segment of cell 1 that contains the original cell center will absorb the small segments of cells 4 and 2 to form a new triangular cell. The remaining segment of cell 4 containing its original cell center now becomes an independent pentagonal cell. With these cut-and-absorption procedures, the interfacial cells are reorganized along with their neighboring cells to form new cells with triangular, trapezoidal, and pentagonal...
shapes in a 2D domain. Figure 4-2 shows an example of the cut-cells after re-construction. When the area of a segment is less that half area of a normal cell, it will be absorbed. This maintains a good ratio between the volumes of the cells, and also ensures that the total number of cells remains unaltered. After this procedure, each newly defined cell maintains a unique index and cell center to support the needed data structure.

The original Cartesian grid will now become a mixed grid which includes some original structured grid, and the unstructured grid due to the newly generated irregularly shaped cut-cells. Figure 4-3 is an example of the mixed structured and unstructured type grid obtained after the merging procedure. Any object without sharp edges can be modeled using the current cut-cell techniques.

4.3.3 Calculation of Fluxes for Cut-Cells

Figure 4-4 shows a Cartesian grid with cells which are cut by an interface. The solid squares indicate the centers of cells. Because of the interface, the original $ABCD$ cell with the cell center 1 will absorb the fragment from another cell to form a trapezoidal cell $BCEF$. The original grid line $AD$ is replaced by a section of interface $FE$ and the original faces $CD$ and $BA$ are extended to become $CE$ and $BF$ respectively.

In the finite volume framework, the fluxes (first derivative) at cell faces and the primitive variables at face centers must be known for forming the surface integral. Therefore, in SIMCC it is very important to obtain highly accurate fluxes and primary variables at the interface or cell faces. Consider the flux $f$ of the flow variable $\phi$ across the cell face $CE$ shown in Figure 4-4. One can construct a second-order accurate integration procedure as follows:

$$
\int_{CE} f \, dy = \int_{CD} f \, dy + \int_{DE} f \, dy \approx f_{CD}(y_C - y_D) + f_{DE}(y_D - y_E) \quad (4-12)
$$

where $f_{CD}$ and $f_{DE}$ are computed at the center of the segments $CD$ and $DE$. Getting the value of $f_{CD}$ is straightforward- linear interpolation can be used to obtain the flux with
Flux computations for cut-cells

second order accuracy:

\[ \phi_{CD} = \phi_1 \lambda_1 + \phi_3 (1 - \lambda_1) \]
\[ \lambda_1 = \frac{x_1 - x_{AC}}{x_1 - x_3} \]

If \( f_{CD} \) represents the normal gradient of flow variable \( \phi \), it can be approximated by the following central difference scheme:

\[ \left( \frac{\partial \phi}{\partial x} \right)_{CD} = \frac{\phi_1 - \phi_3}{x_1 - x_3} \] (4–13)

The above equations cannot be used to estimate \( f_{DE} \), because one of the neighboring cell centers is located on the other side of the interface in a different phase. Also, the center of segment \( DE \) is not located on the straight line connecting the two cell centers. In order to maintain a second-order accuracy, a two-dimensional polynomial interpolating function for \( \phi \) is adopted in the computation of flux for such kind of small segments. An appropriate functional form for \( \phi \) that is linear in \( x \) direction and quadratic in \( y \) direction is given as:

\[ \phi = c_1 xy^2 + c_2 y^2 + c_3 xy + c_4 y + c_5 x + c_6 \] (4–14)
The six coefficients $c_1$ to $c_6$ can be obtained by evaluating $\phi$ at the six points 1 to 6 shown in the Figure 4-4. Thus the variable $\phi$ at the center of the face $DE$ can be expressed as

$$\phi_{DE} = c_1 x_{DE} y_{DE}^2 + c_2 y_{DE}^2 + c_3 x_{DE} y_{DE} + c_4 y_{DE} + c_5 x_{DE} + c_6$$

and the normal gradient can be found from differentiating this expression:

$$\left( \frac{\partial \phi}{\partial x} \right)_{DE} = c_1 y_{DE}^2 + c_3 y_{DE} + c_5$$

(4–15)

A similar approach is used to compute the flow variables or their normal gradients on the remaining segments. Once the primitive variables and the derivatives at all the modified faces have been determined, the coefficients of matrix for the cut-cells can be modified based on this information and the solver will be invoked to obtain the solution.

It must be emphasized that the equation obtained above is only for this specific case. The interpolation polynomial is quadratic in $y$ direction and linear in $x$ direction. For a different interface configuration, the polynomial may be quadratic in $x$.

4.4 Moving Interface Algorithm

For fixed interface problems the techniques discussed up to this point constitute all the elements required to obtain the solution. However, for most problems in multiphase flows, the interface is not fixed and therefore an algorithm to deform the interface to satisfy stress balance is necessary. The moving interface algorithm in this research includes two functions. The first one is to advance the interface [38] and the second one is to update the cells because of change of phase [66].

4.4.1 Interface Motion Due to Stress Imbalance

In unsteady computations, the interface will translate and/or deform to satisfy the interfacial dynamics at each time step. In SIMCC, a ‘push and pull’ strategy first proposed by [38] is used to determine the new location of the interface in order to satisfy the force balance at the interface. The stresses acting at the interface can be divided into the normal and tangential components. In these flow computations, the Reynolds number
being very high, the tangential shear stresses are quite small. Therefore the displacement of interface is governed only by the normal forces at the interface. The new location of interface is determined iteratively. In each iteration, the residual of the force balance in the normal direction will be computed and the displacement of marker points is assumed proportional to this residual:

\[
\begin{align*}
X_{\text{new}}^{n+1} &= X_{\text{new}}^n + \beta_M \cdot \Pi_{n+1}^n \cdot n_x \\
Y_{\text{new}}^{n+1} &= Y_{\text{new}}^n + \beta_M \cdot \Pi_{n+1}^n \cdot n_y
\end{align*}
\]  

(4–16)

where \((X,Y)\) are the coordinate positions of marker points, \((n_x,n_y)\) are the components of normal vector in the \(x\) and \(y\) direction, respectively, \(\Pi\) is the residual of the force balance in the normal direction and \(\beta_M\) is a relaxation factor and it has an empirical value normally in the range of 0.01-0.0001 in this research.

Figure 4-5 illustrates for this interfacial advancing process. In Figure 4-5, a marker point \(A_o\) is located at the initial interface and the residual of force balance in the normal direction \(\Pi_1\) will be computed. Based on the location of \(A_o\) and the value of \(\Pi_1\), the marker point will be pushed to \(A_1\). In this moment, the residual of force balance in the normal direction will be checked. If the new residual \(\Pi_2\) is still large, the marker point \(A_1\) will be pushed to \(A_2\). Once the residual is small enough which means that the force balance in the normal direction has achieved convergence, the iteration will be stopped.
and the normal component of interfacial velocity is found by

\[ u_{new} = \frac{(X_{new} - X_{old})}{\Delta t} \]

\[ v_{new} = \frac{(Y_{new} - Y_{old})}{\Delta t} \] (4-17)

In this iterative procedure, the residual of the force balance in the normal direction is required to be less than 1.0E-3. The normal component of the interfacial velocity will be the velocity boundary condition during the computation. This algorithm is only for the problems without phase change. With phase change, an additional component is added to account for the change in volume due to vaporization.

Figure 4-6. Cell updation procedure

4.4.2 Updating Cells which have Changed Phase

In flow computations with moving/deforming interface, some cells near the interface change their phases after the previous step. In Figure 4-6, the phase of cell center ‘5’ is different from cell called ‘1’, ‘2’, ‘3’ and ‘4’ initially at time \( t \). After the interface moves to the new location at \( t + \Delta t \), the phase of cell ‘5’ will change as the will change as the cell center now lies in ‘Phase 2’. In this case, the fluid properties of cell center will change to the corresponding phase. All new primary variables of cell center ‘5’ should now be obtained by following steps:
1. A normal probe passing through the cell center ‘5’ is taken, and the intersection of this probe with the new interface is denoted by point ‘B’ in the Figure 4-6.

2. The same probe is extended in the opposite direction to locate another point ‘A’ such that the distance between ‘A’ and ‘B’ is $1.5\Delta x$.

3. Find the four cell centers ‘1’, ‘2’, ‘3’ and ‘4’ which surround the point ‘A’. Use the values of the primary variables at these four cell centers and bilinear interpolation to find the value of the primary variables at point ‘A’.

4. Use linear interpolation to obtain the primary variables of cell ‘5’ using their values at points ‘A’ and ‘B’.

5. Update the fluid properties of cell center ‘5’.

Therefore due to the sharp interface method, the values of primary variables ‘jump’ when a cell changes phase. This algorithm is necessary to maintain the consistency of SIM formulation.

### 4.4.3 Interface Motion Due to Phase Change

In this research, because of the large wall superheat phase change is going to take place. Therefore there is mass flux crossing the interface. In order to satisfy the conservation of mass at the interface, the normal velocity is discontinuous at the interface.

As discussed earlier, the normal component of interfacial velocity is determined by the actual interface displacement during $\Delta t$ and the contribution of normal component of interfacial velocity should be determined from both normal force balance condition and phase change:

$$u_{n,int} = \frac{\Delta x_{force-balance} + \Delta x_{phase-change}}{\Delta t} \quad (4-18)$$

where $\Delta x_{phase-change}$ is the contribution from the phase change at the interface. The normal component of interfacial velocity can be expressed as a sum of the two contributions:

$$u_{n,int} = \Delta u_{n,force-balance} + \Delta u_{n,phase-change} \quad (4-19)$$

From conservation of mass at the interface and Eq 4-19, the normal component of the velocity near the interface of each phase can be obtained. The velocities of each phase
are obtained from the conservation of mass at the interface and are discontinuous at the interface to ensure that mass conservation is strictly enforced.

Based on these concepts, the following steps need to be performed to determine the new location of the interface. The total heat flux which causes the phase change near the interface can be expressed as:

$$\dot{q}'' = k_v \frac{\partial T_v}{\partial n} - k_l \frac{\partial T_l}{\partial n} + \dot{q}_{\text{rad}}''$$  \hspace{1cm} (4–20)

The gradients are determined from second order same phase extrapolation. Then the net heat that passes through the interface during the time $\Delta t$ through the area $\Delta A$

$$\Delta e = \dot{q}'' \Delta A \Delta t$$  \hspace{1cm} (4–21)

Therefore the amount of vapor mass produced locally can be given by

$$\Delta m = \Delta e / \lambda$$  \hspace{1cm} (4–22)

From the mass change one can calculate the corresponding volume change of the liquid. This would be the total change in the volume of the liquid phase, and the new position of the interface should satisfy this condition. The marker points are given a local displacement in proportion to the local heat flux versus the total heat flux. The new position is determined iteratively by giving small increments in the normal direction

$$X_{\text{phase-change}} = X_o + \beta_H \cdot n_x$$  \hspace{1cm} (4–23)

$$Y_{\text{phase-change}} = Y_o + \beta_H \cdot n_y$$

where $\beta_H$ is the local mass transfer coefficient and can be calculated from the equations above. Now, a new interface based on the phase change is defined. The next step is to invoke the isothermal moving interface algorithm. Because of the imbalance of force in the normal direction, the new interface will be adjusted again to achieve balance of force in
the normal direction to obtain the final position at each time step.

\[ X_{\text{new}} = X_{\text{phase-change}} + \beta_M \cdot \Pi \cdot n_x \]
\[ Y_{\text{new}} = Y_{\text{phase-change}} + \beta_M \cdot \Pi \cdot n_y \] (4–24)

where \( \beta_M \) is the momentum relaxation factor. This has already been discussed earlier in detail. The only difference is that in Eq 4–24 an initial displacement due to the phase change has already been applied before the iteration starts. In each time step, the total displacement is given as the difference between the original interface position and the final interface position. Therefore, the new normal component of interfacial velocity can be obtained by:

\[ u_{x,\text{int}} = \frac{(X_{\text{new}} - X_{\text{old}})}{\Delta t} \]
\[ u_{y,\text{int}} = \frac{(Y_{\text{new}} - Y_{\text{old}})}{\Delta t} \] (4–25)

In isothermal multiphase flows, the normal component of the interface velocity is equal to the normal component of the phase velocities at the interface. However, because of phase change, the phase velocities would be different from the interface velocity. The normal component of velocity of the two phases should be corrected as

\[ u_{n,l} = \frac{\rho_l u_{n,\text{int}} + \dot{m}''}{\rho_l} \]
\[ u_{n,v} = \frac{\rho_v u_{n,\text{int}} + \dot{m}''}{\rho_v} \] (4–26)

### 4.5 Challenges in Direct Numerical Simulation of Internal Two-Phase Flows with Phase Change

The issues of phase change computations on Cartesian grids have been discussed at some length in [7]. He emphasizes the importance of obtaining accurate mass transfer generated at the interface, for which accurate calculation the heat fluxes is crucial. In this regard, SIMCC is able to perform better than continuous interface methods (CIM) because of its treatment of the interface as an entity with zero thickness, which is much closer to the theory of continuum.
In this work, some problems of phase change computations that are specific to internal flows will be addressed in detail. Internal flows are those which are confined inside a particular geometry, for example, a pipe, a channel etc. External flows are usually those around objects and not confined by any kind of walls. External flows are more easy to simulate numerically because mass conservation is easier to satisfy. The domain can be made sufficiently large to satisfy the far-field boundary conditions. In internal flows, mass conservation is important because of the finite area of inlets and outlets. In internal flows, often the only thing that is known about the velocity at the outlet is the mass flow rate. If the problem is pipe or channel flow, the domain should be made long enough (for laminar pipe flow the entrance length is given by $L_e/D > 0.06Re$ \cite{57}) so that the flow can become fully developed. However, none of these characteristics of internal flows pose any serious problems for single phase simulations.

In multiphase internal flows with phase change, the situation is extremely complicated since the problem is \textit{highly unsteady}. In the context of the inverted annular flow encountered in cryogenic chill down process, the advancement of the liquid phase in the pipe constantly pushes out the vapor, and the area occupied by the vapor phase decreases continuously. No matter what length of the pipe is taken, it will ultimately violate the fully developed boundary condition at the outlet because of the constant decrease in the length of the vapor column. So the simulations need to be stopped after the fully developed condition cannot be satisfied at the outlet. It becomes important to estimate the length of the computational domain, which is difficult to do apriori because even the Reynolds number of the vapor phase is continuously increasing because of phase change. If the length is underestimated, one would not be able to carry out the simulation to its desired conclusion, whereas if it is overestimated, it will unnecessarily slow down the computations.

The geometry of cryogenic inverted annular flow also poses some unique numerical challenges, even though it is one of the simpler flow regimes of those encountered in
two-phase flows. The issue is that the gap between the liquid core and the hot tube wall is extremely narrow. This creates problems in two ways: because of the proximity of the wall, most of the phase change happens in this region, secondly due to the high mass transfer rate, a localized region of very high velocity is created, since all the liquid mass which gets converted into vapor has to be convected out of this constricted space. The high velocities and steep gradients in the vapor phase in this zone create numerical stability issues as the simulation progresses. This is especially true for the current scheme which uses central differencing for the convective term in the momentum transport equation. These issues are illustrated in Figure 4-7. The narrow high vapor velocity region shown in the figure which is due to the slight bulge in the advancing liquid front will henceforth be referred to as the ‘bulge’ region.

To address these concerns in the simulation of two-phase internal flows, it is proposed to take the following actions. First and foremost, there is a real need to increase the performance of the current SIMCC code to enable high accuracy calculations of larger domains than can currently be handled. Therefore, multigrid acceleration techniques become a necessity. Multigrid methods are very efficient and can solve a discrete system.
of $n$ equations to the desired accuracy in $O(n)$ computer operations [68]. Secondly, it is extremely important to address the numerical issue of convective instability due to the high vapor velocity and gradients in the ‘bulge’ region. Therefore, it is proposed to use an upwind differencing scheme to mitigate the convective instability effects [60, 69]. The specific scheme suggested is the modified QUICK by [70], which is a stable and fast converging variant of the original QUICK scheme by [71]. All of these methods will be discussed in more detail in the following sections.

4.6 Multigrid Method for SIMCC

As discussed in the previous section, numerical simulation of multiphase flows with phase change poses several challenges. To address these concerns, there is a strong stimulus to increase the efficiency of the present numerical techniques by using multigrid acceleration techniques.

It is well known that in the solution of Navier-Stokes equation, the slowest equation to converge is the elliptical pressure equation. One effective way to speed up the convergence is to use multigrid methods. Research in multigrid methods started in the 1960’s. The first paper on multigrid methods was by [72] and addressed the solution of pressure-Poisson equation on a unit square. Since then, the research in multigrid methods has proceeded at a rapid pace. A few notable works in this regard are [68, 73–75]. Multigrid methods are now used to solve a wide range of linear and nonlinear boundary value problems. Multigrid methods are very efficient and can solve a discrete system of $n$ equations to the desired accuracy in $O(n)$ computer operations [68]. In the recent years, some researchers have developed multigrid techniques for multiphase flows [65, 76, 77]. However, most researchers use the Algebraic Multigrid method (AMG) which ignores the presence of the interface on the coarser grids. Since the SIMCC makes use of an ordered but possibly non-uniform (but with no fine grid ‘patches’) and unstructured grid, it is possible to implement a geometric multigrid scheme for SIMCC.
4.6.1 The Multigrid Technique

The basic idea behind multigrid methods is based on the property of certain iterative solvers (Gauss-Siedel, Jacobi, SOR) to rapidly reduce the high frequency errors, but giving slow convergence for low frequency errors relative to the grid size. Therefore, on a fine mesh, these solvers initially show a rapid decrease in the residuals, followed by a very slow convergence rate. This property of the iterative solvers is known as ‘relaxation’, and these solvers are also known as ‘relaxers’. Relaxers tend to smooth out the high frequency errors. Multigrid methods make use of this property of the relaxers by defining coarser grids on which a low frequency error will be seen as a high frequency one. Consider a large sparse system of equations given by

\[ A_n u = f_n \]  (4–27)

where \( A_n \) is an \( n \times n \) matrix. After a certain number of iterations, let the error in the approximation \( \tilde{u} \) be denoted by \( e_n \). Then the error satisfies the modified equation

\[ A_n e_n = r_n = f - A_n \tilde{u} \]  (4–28)

where \( r_n \) is called the residual. Since the error \( e_n \) is smooth after the relaxation sweeps, therefore the residual \( r_n \) is also expected to be smooth. The idea is to solve the modified Eq 4–28 on the coarse grid. For this purpose, the residual is ‘restricted’ onto the coarser grid.
grid by the restriction operator $\mathcal{R}$. This is shown symbolically in the Figure 4-8, where three grid levels have been taken for illustration.

$$r_{n-1} = \mathcal{R}(r_n) \quad (4-29)$$

The error is found by solving the modified equation on the coarser grid and then applied as a correction to $\tilde{u}$ on the fine grid after prolongation, denoted by the operator $\mathcal{P}$.

$$A_{n-1}e_{n-1} = r_{n-1} \quad (4-30)$$

$$u' = \tilde{u} + \mathcal{P}(e_{n-1}) \quad (4-31)$$

The idea can be extended to multiple grid levels by using recursion. The key elements in developing the multigrid solver appropriate to a specific problem are the restriction and prolongation operators and choosing the scheme for approximating the matrix $A_n$ on the coarser grids. An enhancement to this basic approach is provided by solving the equation

$$A_ku_k = f_k \quad (4-32)$$
on the coarse grid first, where $f_k$ is again found by restriction of $f_n$. This provides a better initial guess for $u$ on the fine grid. This is known as the full multigrid or FMG.

### 4.6.2 Implementation of Multigrid Method for SIMCC

In the current code, the fractional step method is used to solve the momentum equations. This involves the solution of the pressure equation over the regular Cartesian grid in the bulk and cut-cells in the interfacial region. Near the interface there is a sharp jump in the pressure due to the surface tension, leading into potential non-linear situation, especially when phase change is also involved. Therefore it becomes necessary to consider the details of the interface when designing $\mathcal{R}$, $\mathcal{P}$ and the matrix approximation $A_k$ (where $k$ represents coarser grid levels) if better stability is desired.
Based on these considerations, the coarse grid matrix $A_k$ will be obtained by discretizing the partial differential equation on the coarse grid. This is known as the *discretization coarse grid approximation* [78]. Figure 4-9 shows a typical case. In the figure, the fine grid is shown by the lighter color lines, while the coarse grid is superimposed in a darker hue. The centers of the coarse grid control volumes shown by square shaped points fall at the intersection of the fine grid lines. The cell centers of the fine grid are shown by lighter dots. The figure shows a few cut-cells formed by the coarse grid which are shaded and marked $a$ and $b$. For regular cells like $c$, four fine grid cells form a single coarse grid cell. The matrix $A_k$ would be formed by discretizing the pressure equation on this coarse grid:

$$- \int_{cs} (\bar{\nabla} p^{n+1}_k) \cdot \bar{n} \, dS = \frac{1}{\Delta t} \int_{cs} (\bar{U}_k^* \cdot \bar{n}) \, dS \quad (4-33)$$

For a regular cell in the bulk phase, this would lead to an expression like:

$$p_P \left( 2 \frac{dy_k}{dx_k} + 2 \frac{dx_k}{dy_k} \right) - p_E \frac{dy_k}{dx_k} - p_W \frac{dy_k}{dx_k} - p_N \frac{dx_k}{dy_k} - p_S \frac{dx_k}{dy_k} =$$

$$- \frac{1}{dt} \left[ (U_{x,E}^* - U_{x,W}^*) \, dy_k + (U_{y,N}^* - U_{y,S}^*) \, dx_k \right] \quad (4-34)$$

Here $dx_k, dy_k$ denote the grid spacing for the coarse grid $k$. Thus, only the source term is different for a regular cell, the matrix remains the same since the ratio of $dx_k, dy_k$ remains the same for the coarse grid. Cut-cells and cells near boundaries will have other contributions arising from the interfacial and boundary conditions respectively.

The prolongation and restriction operators for a regular cell are calculated using simple bilinear interpolation. In Figure 4-9, it can be seen that for every fine-grid cell in the bulk, denoted by gray dots, there can be found four coarse-grid cell-centers in the same phase surrounding it. The same is true for coarse-grid cell centers away from the interface - there can be found four fine-grid cell centers around it which are in the same phase. These four points are used to construct a bilinear polynomial for restriction or
prolongation. For cells which do not have all the neighboring points in the same phase, special one sided interpolation needs to be performed.

Figure 4-9. Illustration of the multigrid technique for SIMCC

4.6.3 Treatment of Cut-Cells on Coarse Grid

To formulate the matrix $A_k$ on the coarse grid, we need to know the contribution from the interfacial conditions. This requires many calculations to be performed for the coarse grid. However, one need not calculate all the geometrical information anew for the coarse grid cut-cells. This is because the normal, curvature and phase have already been determined for the fine grid. This information can be manipulated and used with coarse grid cut-cells.

For example, to determine the phase of a coarse grid cut-cell, the information about the phase of fine grid cells can be utilized. In Figure 4-10, it can be seen that a coarse cell is superimposed on four fine grid cells, labeled ‘a’, ‘b’, ‘c’ and ‘d’ in the clockwise direction from the top-left corner. These cells have the phase ‘1’ or ‘0’ depending on whether they are in the immersed phase or mother phase, respectively. To determine the phase of the coarse-grid cell, we construct a variable from the values of a, b, c, d. Essentially, this variable stores the information about the phases of the four fine grid cells, and may be called ‘abcd’. This information can be parsed to determine the phase and type of the coarse-grid cut-cell. If all four cells have the same phase, i.e., ‘abcd’ is either ‘1111’ or ‘0000’, then it
can be deduced that the coarse grid control volume belongs to the same phase, either ‘1’ or ‘0’. If three cells have same phase, then the phase of the bigger cell is determined from the phase of the majority of the smaller cells. Special second order one-sided interpolation is needed to determine the properties or residual at the cell center of the coarse cell in restriction. Lastly, if two cells have same phase, then phase of the bigger cell needs to be determined carefully from interface location. Second order one-sided interpolation is needed for restriction of the residual from the fine grid.

Figure 4-10. Determination of the phase of coarse grid cut-cells

After the restriction operation (Eq. 4–29), one needs to formulate the matrix $A_k$ on the coarse grid. Regular cells are treated as discussed in the previous section. For cut-cells, it is important to reorganize them into a consistent mosaic using the merging procedure. So exactly the same set of calculations need to be performed as for the fine grid discussed in Section 4.3.2 and 4.3.3. After this procedure, the Eq. 4–30 can be solved on the coarse grid to get $e_k$.

The prolongation operator (Eq. 4–31) also uses information from the fine grid wherever possible, and is designed to honor the presence of the interface. Prolongation is the inverse operation, where the solution from the coarse grid cell and its neighbors lying in the same phase will be used for linear interpolation at the fine grid cell centers. However, now four
coarse grid cells surround four fine grid cells as can be seen from Figure 4-9. Therefore, this situation is more complex than restriction, but the approach towards polynomial interpolation is similar. Only cells from the same phase will are used for the interpolation, and one sided interpolation is needed for many cut-cells.

4.6.4 Results with Multigrid

The efficiency of the multigrid method was first tested the pressure-Poisson equation solver without the cut-cells first. The test was performed using the benchmark case lid driven cavity flow for single phase. In Figure 4-11, $Re = 100$, $dt = 0.01$ and a $128 \times 128$ grid has been used. It is seen that there is a significant advantage obtained by using multigrid both in terms of the CPU (central processing unit) time and the number of iterations on the fine grid. For grid levels greater than two, the number of iterations on the fine grid remains almost the same, but there is still a significant decrease in the CPU time as seen in Figure 4-12.

![Figure 4-11. Efficiency of multigrid based on number of iterations](image)

Next, the geometric multigrid scheme for SIMCC was tested with an artificial interface embedded in the lid driven cavity flow. This tests the multigrid subroutines which handle the cut-cells near the interface, such as restriction and prolongation for
Figure 4-12. Efficiency of multigrid based on CPU time

coarse grid cut-cells described in Section 4.6.3. The interface has a radius $R = 0.1$ and is located at the center of the cavity which is a unit square. The viscosity and density of the phases both inside and outside the artificial interface are set as equal. The set up of the problem is similar to that used by [65] to test their multigrid method. The boundary conditions at the interface are normal stress balance, shear stress balance and the pressure is same on both sides of the interface. The simulation was done for $Re = 100$, $dt = 0.01$ and a $128 \times 128$ grid as before. Two grid levels are used for the results that follow, one is the fine grid with spacing of $\Delta x = \Delta y = 0.007813$ and another coarser grid with $\Delta x = \Delta y = 0.015625$.

Figure 4-13 shows the streamlines for the baseline case which is simple lid-driven cavity flow without interface and without multigrid, and the test case with embedded artificial interface and multigrid. This tests the accuracy of cut-cells routines as well as the multigrid routines. It can be seen that the streamlines closely match. The effect of the interface on the streamlines in Figure 4-13B is minimal. The streamlines pass through the interface without any distortion or bending. This shows the high level of accuracy possible with the current geometric multigrid method coupled with SIMCC procedures.
Figure 4-13. Streamlines with and without artificial interface

Figure 4-14. Centerline velocities with and without artificial interface

To further compare the velocities, the $u$-velocity on vertical centerline and the $v$-velocity on horizontal centerline are shown in Figure 4-14 for the same two cases. The velocity calculated with multigrid method and artificial interface is shown by the dashed line. It
is seen that the velocities are almost indistinguishable from the velocities for the baseline case.

Figure 4-15 shows the performance of multigrid for the test case of lid driven cavity flow with artificial interface. The baseline case for this is artificial interface problem without any multigrid acceleration, solved using only the SIMCC techniques. The residual is plotted on the y-axis. It can be seen that both in terms of the fine grid iterations and the CPU time, multigrid (2 level V-cycle) far outperforms SIMCC without multigrid enhancement. Without multigrid, SIMCC takes about 540 seconds to reduce the residual by four orders of magnitude. With multigrid acceleration, this operation only takes about 200 seconds. This is an improvement in speed by a factor of more than 2.5, maintaining the same level of accuracy.

4.7 QUICK Differencing Scheme for the Convective Term

In the present numerical scheme, central differencing scheme (CDS) has been used to discretize the convective term in the advection-diffusion step of the fractional step method. Although CDS has many strengths for application to general flow situations (conservativeness, second order accuracy etc., for properties of numerical differencing
schemes see [69]), it also has certain drawbacks when applied to internal flow situations. The reason is that CDS does not recognize the direction of flow or the strength of the convection term relative to the diffusion term.

![Diagram of QUICK discretization of convective term](image)

Figure 4-16. Schematic for QUICK discretization of convective term

In general, the convective term for any intensive fluid property \( \varphi \) can be discretized as:

\[
\int_{cs} \varphi (\vec{u} \cdot \vec{n}) \, dS = \varphi_e F_e - \varphi_w F_w + \varphi_n F_n - \varphi_s F_s
\]  

(4–35)

where \( \varphi = \{u, v, T\} \), \( F \) represents the velocity flux at the cell face calculated as \( F = (\vec{u} \cdot \vec{n}) \Delta s \) and the subscripts \( e, w, n, s \) denote the east, west, north and south faces of the control volume respectively. In CDS, \( \varphi_e \) is calculated as an average of the values at the cell centers \( E \) and \( P \). Thus it gives equal weightage to the node upstream and downstream of the cell face. An upwind scheme gives more weightage to the upstream node. For a flow situation where convection is relatively strong, the downstream node has a minimal influence on the flow upstream. Therefore, upwind schemes are more suited to handle certain types of flows. This property of a differencing scheme to recognize the flow direction is known as transportiveness. \( Pe_{\text{cell}} \) is a non-dimensional number that relates the strength of the convective term to that of the diffusion term. CDS is said to lack transportiveness for high \( Pe_{\text{cell}} \), where

\[
Pe_{\text{cell}} = \frac{\rho u \Delta x}{\mu}
\]  

(4–36)
The mechanism by which CDS creates problem is by giving negative coefficients for $Pe_{cell} > 2$, which can produce solutions that oscillate from node to node. These are known as overshoots and undershoots. $Pe_{cell} > 2$ implies that the convective term is stronger as compared to the diffusive term. Thus the coefficient in the matrix equations can become negative. For boundedness of a numerical scheme, the coefficients should all have the same sign [79]. If this can not be satisfied, it leads to physically unrealizable solutions with oscillations.

Upwind differencing schemes give more weightage to the upstream node when calculating the convective flux at the control volume face and are able to alleviate the unboundedness problem to various extents. There are various types of upwind differencing schemes available, including the first order upwind differencing (FOU), the hybrid scheme, the power law scheme, the third order QUICK (Quadratic Upwind Interpolation for Convective Kinematics) scheme made popular by [71] etc. FOU scheme is stable for all $Pe_{cell}$ but has lower accuracy than CDS and suffers from false diffusion.

In this research, it is proposed to use a variant of the QUICK scheme by [70] which is more consistently formulated. This scheme has the advantage that it is more stable than the original QUICK scheme and satisfies the requirements of conservativeness, boundedness and transportiveness. It achieves this by placing troublesome negative coefficients in the source term, and retaining only positive coefficients in the main matrix. For a uniform grid, the $x$-direction terms discretized using the QUICK scheme by [70] can be written as:

$$
\varphi_w = \varphi_W + \frac{1}{8} [3\varphi_P - 2\varphi_W - \varphi_{WW}] \text{ for } F_w > 0
$$

$$
\varphi_e = \varphi_P + \frac{1}{8} [3\varphi_E - 2\varphi_P - \varphi_W] \text{ for } F_e > 0
$$

$$
\varphi_w = \varphi_P + \frac{1}{8} [3\varphi_W - 2\varphi_P - \varphi_E] \text{ for } F_w < 0
$$

$$
\varphi_e = \varphi_E + \frac{1}{8} [3\varphi_P - 2\varphi_E - \varphi_{EE}] \text{ for } F_e < 0
$$

(4–37)

where the subscripts $P, E, W, EE, WW$ indicate the cell, and its east, west, far east and far west neighbors respectively. The convective term is now handled implicitly. Only
the contribution from the immediate upwind node is retained in the matrix, the term in square brackets is lumped with the source term. Therefore the coefficient matrix for this scheme is the same as FOU. Similar expressions can be written for the contributions from the $y$-direction. For a non-uniform grid, the above expression needs to be generalized. Since three nodes are used in the calculation, therefore we can use a quadratic fit to calculate $\varphi$ at the cell face:

$$
\varphi = ax^2 + bx + c \quad (4-38)
$$

where points 1, 2 and 3 denote the three consecutive points needed to evaluate $\varphi$- $W$, $P$ and $E$ cell centers for example.

Since this scheme stores the negative coefficients in the source term, and treats convective term implicitly, the computational effort is expected to increase somewhat. The time step also needs to be smaller than for CDS. However, this scheme enhances the stability of the computations significantly, and delays the onset of numerical instability associated with the non-linear convective term. This strategy is also known as the deferred-correction approach [60]. Another reason to do this is to avoid getting a very large computational molecule, which would happen if all the terms were treated implicitly.

Figure 4-17 shows some simulation results with CDS and QUICK. In Figure 4-17A, $Pe_{cell} > 2$ and CDS creates oscillations shortly afterwards. In Figure 4-17B, $Pe_{cell} > 4.5$ but QUICK scheme is still stable. In fact, it was possible to run almost all of the cases for $Pe_{cell} > 8.0$, without changing the grid spacing. This shows that the QUICK scheme is very effective in improving the stability of the code due to the convective term.
Figure 4-17. Comparison of convective schemes
In this chapter, the SIMCC with moving interface algorithm is tested thoroughly through a series of test cases of increasing difficulty level. Not only numerical test cases but also actual physical problems have been studied. Results from the SIMCC code have been compared against analytical, numerical and experimental results for standard(benchmark) problems by various researchers.

The first case is a benchmark problem for testing any 2D Navier-Stokes solver: the lid driven cavity flow. Tests have been done for a range of Reynolds numbers from 100 to 5000. The second test case is that of a flow over a sphere, which is selected for testing the cut-cell algorithms for handling a stationary interface. Various features of the flow have been calculated, including the drag on the sphere, as a function of $Re$ in the range of 1 to 100. The third test case is the isothermal bubble moving in a pool in a gravitational field. The interface in this validation case will not be stationary but moving and deforming and therefore a moving interface algorithm must be imported to handle the movement of the interface. The fourth and last test case is the Bretherton problem with gas finger moving in a channel filled with a liquid. This case is very close to the inverted annular film boiling geometry. In all of the cases, tests have been performed for a range of the critical parameters like $Re$ and $We$.

5.1 Test Case 1: Lid Driven Cavity Flow

Lid driven cavity flow is a well documented problem and can be used as a validation case for 2d Navier-Stokes code. It has simple geometry and simple boundary conditions. Since this problem is very well documented, there is a lot of data available for comparison. A well accepted set of data for comparison is the data of [80], since it includes tabular results for various Reynolds numbers. It is also gives data for a wide range of $Re$. They use the stream function and vorticity formulation. Therefore, we have chosen this test case to benchmark our code.
The geometry consists of a square or rectangular cavity, with Dirichlet boundary conditions on all sides. The top moving wall is given a unit velocity, which drives the flow. The present code implements the finite volume discretization and the fractional step algorithm to solve the Navier Stokes equation in a non-staggered grid. It was tested for accuracy at various Reynolds numbers between 100 and 5000. Iterations were performed until convergence was reached when the velocity and pressure residuals became less
than 1.0E-8. In Figure 5-1, the $u$ velocity at the vertical center line has been plotted. Figure 5-2 shows the $v$ velocity at the horizontal center line. Both the cases have been plotted against results of [80]. The velocity plots have been staggered by 0.2 units along the $y$ axis for better clarity. Grid resolution of $64 \times 64$ has been used for Reynolds numbers up to 1000, and the results agree well with [80]. At higher Reynolds numbers, the results with a $64 \times 64$ grid were not found to be accurate enough. Therefore, a finer grid of $128 \times 128$ has been used. In all the cases, the pressure and velocity residuals had reduced to less than 1.0E – 8. The results show good quantitative agreement with the benchmark data. Figure 5-3 shows the streamline plots for the cases $Re = 100$ and $Re = 400$.

5.2 Test Case 2: Flow Over a Solid Sphere

Axisymmetric, laminar, steady flow over a sphere is studied. This problem tests the cut cell algorithm employed for solving flow over an arbitrary smooth surface. Various parameters like wake length, vortex center, and coefficient of drag were calculated and compared with numerical and experimental results for the Reynolds number in the range of 1 to 100. Above Reynolds number of about 130, the flow becomes unsteady and
vortex shedding occurs [81]. Hence, we have restricted ourselves to this range of Reynolds number.

The computational domain is $15d$ in length and $5d$ in width, where $d$ is the sphere diameter. On the left boundary, a unit inlet velocity is prescribed. The lower boundary is symmetric due to the assumption of axisymmetry. The far-field boundary condition must
be used for the top and right boundary for accurate results. A uniform grid resolution of 0.05 has been used. This grid spacing was chosen on the basis of a grid refinement study.

Simulation was done for Re in the range of 1 to 100. It was found that flow separation occurs at Re=25. This is in agreement with [81] who found an experimental value of Re=24 at which separation occurred. For Re=30 and higher, wake length and the vortex center have been compared with the experimental results of [81]. Figures 5-4A and 5-4B show good agreement both in terms of the trend and the actual calculated values. In Figure 5-5, the calculated coefficient of drag is compared with the numerical results of [82]. The error is found to be within 3 percent for all the six cases. This proves that the present code can calculate the drag over a surface very accurately using SIMCC, and attests to the high accuracy possible with SIMCC. Therefore, from this test case we can conclude that the techniques for handling the stationary interface including the governing equations solver and SIMCC are sufficiently verified.

5.3 Test Case 3: Deformable Bubble Moving in Quiescent Liquid Pool Under Gravity

In the third test case, the buoyancy-driven rising bubble in a quiescent liquid is studied. It tests the accuracy of the moving interface algorithm in conjunction with
the cut-cell algorithms. Some of these results have been published [83, 84]. This case conclusively proves the ability of the present code to handle deformable interfaces in two-phase flows with high accuracy.

In this computation, water is adopted as the ambient liquid and the isothermal bubble contains water vapor at the same temperature as the liquid, so the density ratio 0.0006 and viscosity ratio is 0.045. The range of Reynolds numbers investigated is $1 < Re < 100$, and that of Weber number is $1 < We < 10$. The entire flow is assumed to be axisymmetric and incompressible, with constant properties. There is no heat or phase change mass transfer in this problem. The assumption of axisymmetry allows us to use 2d Navier Stokes equation in cylindrical coordinates. The hydrostatic and dynamic pressures are assumed to be decoupled. The former is computed as a function of the distance from the free surface whereas the latter is computed during the main flow simulation.

Since this is an axisymmetric computation, a rectangular domain with a length of $58d$ and a width of $38d$ is used to simulate an unbounded liquid pool. This size of the domain was found to satisfy the far-field boundary conditions which require all the gradients to go to zero. A graded mesh has been used in both $x$ and $y$ directions, with the mesh becoming progressively refined near the section where the bubble motion and wake formation occurs. The grid is 300x100, with a grid spacing of 0.04 near the bubble. The simulation is started with an initially stationary liquid pool and a stationary spherical gas bubble of radius 0.5. Gravity acts in the negative $x$ direction, therefore the motion of the gas bubble occurs in the positive $x$ direction due to buoyancy forces.

As for the boundary conditions, the lower boundary is an axis of symmetry for the domain. Hence the symmetry boundary conditions apply. In keeping with the assumption of an unbounded liquid pool, a large domain of computation has been chosen. which can ensure that the velocity gradient in the normal direction would go to zero at the left, top and right boundaries. Hence, the far-field boundary condition is specified on the left, top and right wall. The moving interface algorithm was validated by computing flow around
Figure 5-6. Computed bubble shapes

<table>
<thead>
<tr>
<th>Re</th>
<th>$W_e$</th>
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<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
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</tr>
<tr>
<td>10</td>
<td><img src="image2" alt="bubble shapes" /></td>
</tr>
<tr>
<td>100</td>
<td><img src="image3" alt="bubble shapes" /></td>
</tr>
</tbody>
</table>


the moving and deforming bubble. Results were presented in the form of streamline plots, bubble shape aspect ratio and drag.
5.3.1 Bubble Shape

Simulation was done for \( Re \) in the range of 1 to 100, and \( We \) in the range 1 to 10. The computed shapes have been shown in Figure 5-6. The shapes are in good agreement with those calculated by [39] which are shown in Figure 5-7. Results for \( Re=0.5, We=0.5 \), and \( Re=1.0, We=1.0 \) are given in Figure 5-8, and compared to the shapes calculated for the same parameters using the asymptotic formula of [37]. The solution by [37] has been derived under the assumptions that \( Re << 1, We << 1, \) and \( Re^2 << We \). It can be seen that the agreement between our solution and that given by the asymptotic theory of [37] is very good.

![Figure 5-8. Comparison of bubble shape with asymptotic result by [37]](image)

5.3.2 Shape Transition

Figure 5-9 shows the streamlines in both the phases after the bubble has reached steady state. The shape of the bubbles changes from spherical to oblate spheroid with an increase in \( We \). For \( Re = 1 \), the bubble begins to flatten at the rear end with increasing \( We \), and finally has a sort of indentation at \( We = 10 \). This can be seen clearly in Figure 5-9A. Also, the shape of the bubble does not seem to change much on increasing the \( We \). Looking at Figure 5-6, it can be noted that there is a change in the shape pattern.
Figure 5-9. Transition in shape

of the bubbles between $Re = 10$ and $Re = 100$, for the whole range of $We$ studied. At $Re = 100$, the bubbles begin to have greater deformation at the front end. This becomes more and more obvious as $We$ increases. At $We = 10$ there is actually an indentation at the front end of the bubble. To understand this transition, a case with $Re = 50, We = 3$ is also presented. The results are shown in Figure 5-9C. It is seen that the shape of the bubble is nearly symmetrical. This finding is consistent with the results reported by [39]
who also found that this kind of shape transition occurs for $Re = 100$. They too report that $Re = 50$ is the border line case and seems to have fore-aft symmetry.

To characterize this transition further, the researcher looked at the surface tension distribution on the bubbles for $We = 3$, at the four different $Re$ in Figure 5-10. The
shape of the bubble directly depends on the net surface tension force acting on it. Surface tension is given by the curvature divided by $We$, and since the latter is the same for all the four cases, we can compare the curvature of the bubbles. It is seen that for $Re = 50$, the curvature is nearly the same at the front and rear. This implies that for this case, the normal forces on the front and the rear of the bubble are such that their cumulative effect produces the approximately same surface tension force on the bubble. Also, the highest curvature occurs almost exactly at the center of the bubble, indicating the flattening effect at both the front and rear surfaces. For $Re = 1$, the curvature is highly asymmetrical, indicating that the shape of the bubble too lacks fore-aft symmetry. The curvature is negative at the rear end, because of the indentation. Thus, it is observed that the curvature and therefore the shape of the bubble are a strong function of the Reynolds number.

5.3.3 Bubble Shape Aspect Ratio

In Figure 5-11 the aspect ratio of the bubbles is compared to [85] for $Re = 10$ and 100. The comparison is very favorable. It is seen that the aspect ratio is a very strong function of the Weber number. High $We$ implies weaker surface tension which gives higher deformation, while the limit $We = 0$ corresponds to infinite surface tension and perfectly spherical bubble. The aspect ratio is also influenced by $Re$, higher $Re$ giving higher deformation as well.

5.3.4 Circulation

A region of circulation develops behind the bubble for higher $We$. Figure 5-12 shows the wake behind the bubble for different $Re$. The circulation is just evident at $Re = 1$, while by $Re = 100$ there is a fully formed detached circulation zone behind the bubble.

5.3.5 Time Dependant Drag

Results for the drag on the bubbles are presented. The drag force on the bubble derives from three types of forces: dynamic pressure, normal stress and shear stress. By integrating these forces on the surface of the bubble, we arrive at the pressure drag,
Figure 5-12. Development of circulation region

normal drag and shear drag respectively. The coefficient of drag is defined as follows:

\[ C_D = \frac{8F_D}{\rho U^2 \pi d^2} \]  \hspace{1cm} (5-1)

where \( F_D \) is the drag force, \( d \) is the equivalent diameter of the bubble, and \( U \) is the terminal velocity. The contributions from these three components have been shown in Figures 5-13 and 5-14 for two representative cases. The figures show how the forces on the bubble develop during the unsteady simulation. When the drag on the bubble becomes relatively constant it means that the bubble has reached its terminal velocity and shape. In these computations, the initial drag force on the bubble is not zero. This is because the bubble is initially stationary in a gravitational force field. Therefore in numerical simulations, the ‘push and pull’ strategy attempts to balance this gravitational force on the bubble by the pressure forces.

In the figures, the total drag coefficient matches well with other published results. For \( Re = 10, We = 3 \) we obtain \( C_D = 3.4 \), which compares well with the value of 3.3 calculated by [39]. For \( Re = 100, We = 3 \), [39] predict a value of \( C_D = 0.62 \). In our simulations, we obtain a value of 0.61.

From Figure 5-13 and 5-14, several observations can be made. First of all, it is to be noted that the normal drag and the pressure drag seem to be complementary to each other. At the start of the simulation, since the bubble is stationary, the normal and shear
stress on the bubble are negligible. During the simulation, as the bubble accelerates and deforms the contribution of the pressure forces to the total drag decreases, while the normal and shear forces increase in magnitude. Another feature of the flows is that the contribution of the shear drag to the total drag decreases with increasing Reynolds...
Table 5-1. Drag on deformable bubble

<table>
<thead>
<tr>
<th>$Re \backslash We$</th>
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<th>3</th>
<th>6</th>
<th>10</th>
</tr>
</thead>
<tbody>
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<td>27.34</td>
<td>28.30</td>
<td>23.80</td>
<td>21.22</td>
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<td>0.42</td>
<td>0.62</td>
<td>1.23</td>
<td>2.77</td>
</tr>
</tbody>
</table>

number. At $Re = 10$, it is found that shear drag is responsible for almost ten percent of the total drag. At $Re = 100$, this contribution drops to about four percent. This finding is consistent with the physics of the problem, since the viscous stresses are lower at higher $Re$. Also note that the contribution of the normal viscous stresses is significantly reduced with increasing $Re$. At $Re = 10$, pressure and normal drags seem to have an almost equal contribution to the total drag on the bubble, but at $Re = 100$, the normal drag is only about twenty percent of the total drag. In fact, at $Re = 100$, pressure drag dominates, and this trend is similar to what is observed with flow over rigid spheres.

In Table 5-1, we show the results for the total drag on the bubble. The range for Reynolds numbers investigated is $1 < Re < 100$, and that of Weber number is $1 < We < 10$. The first line for each case shows results from SIMCC. The second line shows results by [38, 85]. The results with no footnote correspond to [38]. It is seen that the results are in good agreement with those by [38, 85], except for the case where $Re = 1$. This is a weakness of the present interfacial advection technique, that can satisfy the stress balance at the interface in an approximate manner. This is a problem only for very low $Re$

---

1 Lai et. al.(2003)
(\(Re \leq O(1)\)) flows in which the viscous stresses are substantial. In simulation of cryogenic chill down process, such a situation would never be encountered. Moreover, since the error in the computations is of second order, it is mainly the drag force which is affected. The shape calculations are not affected by these second order errors.

### 5.4 Test Case 4: Bretherton Problem

A classical multiphase problem is that of an elongated air bubble steadily displacing the liquid between two closely spaced parallel plates. As the air bubble moves into the liquid phase, it leaves behind a thin film of liquid at the wall. This is called the Bretherton problem or liquid plug flow and is used as a benchmark case for two-phase fluid infused type problem in a channel or tube. For low \(Ca\), it is found that the film thickness is a function of only the \(Ca\). This problem has been studied extensively by researchers [32–35, 86, 87]. This problem can be used for validation of our numerical method since the geometry is very similar to the cryogenic chill down flow in pipes, the only difference being that this is an isothermal multiphase flow. The work of [35] has been selected to compare the results.

The schematic of the problem is shown in Figure 5-15. In the reference frame fixed to the walls, this problem is inherently an unsteady problem due to the translation of the air bubble. If however a moving reference frame attached to the tip of the air bubble is selected, it transforms into a steady state problem. Since the air channel is infinite in both directions and the air-finger also extends to negative infinity, this can be done. In the original reference frame if the terminal velocity of air bubble was \(U\), then in the new reference frame the top wall translates at a velocity \(u = -U\). The gas phase remains stationary and has constant pressure. At both the left and the right boundaries, the \(x\)-gradients of velocity are negligible since the flow is fully developed. The interface is assumed to behave like a free surface with zero normal velocity. Plug flow can be assumed near the left boundary. Since the flow field is symmetric only the upper half is modeled. The bottom wall is given the symmetry boundary condition whereby gradients and
velocity in the $y$-direction are zero. The problem is non-dimensionalized using the channel half width $H$, the bubble velocity $U$ and the liquid’s properties as reference. The inertial scale is used for pressure. The pressure at the right boundary is selected as reference and set to zero. The non-dimensional parameters of interest are

$$
Re = \frac{\rho_l U H}{\mu_l}, \quad Ca = \frac{U \mu_l}{\sigma}, \quad We = \frac{\rho_l U^2 H}{\sigma}
$$

The computational domain consists of a rectangular area with non-dimensional units of $L = 20$ and $H = 1$. The initial shape of the interface is constructed from a straight line and a half circle, with the tip of the interface being fixed at $x = 3.0$. During the course of simulations, the shape of the bubble changes as the flow field develops around the bubble. Pressure in the gas phase is also calculated during the numerical procedure.

Figure 5-15. Setup for Bretherton problem

Figure 5-16 shows the pressure contours and streamlines when steady state is reached. The final position of the interface is $y = 0.8838$ at $x = 0$. This corresponds to a film thickness of $h_o = 0.1162$. This compares well with the value calculated by [35], $h_o = 0.123$ with less than six percent error. There is a vortex formed near the tip of the bubble. The pressure on the top wall ($y = 1.0$) is shown in Figure 5-17. The reference level for pressure is shifted to the downstream location $x = 13$ and it is multiplied by the Reynolds number to compare with [35]. The pressure distribution shows both qualitative and quantitative agreement. In the results by [35], the pressure near the inlet is The pressure stays relatively constant in the film region near the left boundary because the velocity
profile there nearly corresponds to plug flow. There is a sharp drop in the pressure near the bubble tip in the vortex region, followed by a constant gradient zone near the right boundary. This is explained by the Poiseuille velocity profile which develops in the region near the channel exit. In the plug flow region where pressure is nearly constant, [35] reports a pressure of \(P_{wall} = 49\) for \(Ca = 0.05\) and \(Re = 0\) and \(P_{wall} = 55.4\) for \(Re = 70\).

In our test case, we obtain \(P_{wall} = 52.5\) for \(Re = 10\) and \(Ca = 0.05\). Figure 5-18 shows the values of film thickness obtained for three different \(Ca\) - 0.05, 0.1 and 0.25. The results have the same trend as [35] and are within seven percent for all the cases.

5.5 Conclusion

In this chapter, the ability of SIMCC to handle arbitrarily shaped interfaces, both rigid or deformable, has been established. The drag results for flow over a solid sphere and a deformable bubble fully demonstrate the high accuracy with which SIMCC can treat interfacial dynamics. The Bretherton test case shows that SIMCC can handle internal two-phase flows with accuracy. Therefore in the class of sharp interface methods, SIMCC presents an alternative to methods that use body-fitted adaptive grids [38, 40, 85] for simulating multiphase flows.

Figure 5-16. Flow field and pressure contours for \(Re = 10, Ca = 0.05\)
Figure 5-17. Pressure at the channel wall for $Re = 10, Ca = 0.05$

Figure 5-18. Film thickness for $Re = 10$ and different $Ca$
6.1 Scope of Cryogenic Chill Down

In this chapter, cryogenic chill down of liquid nitrogen, oxygen and argon involving phase change has been studied. Cryogenic fluids commonly used are nitrogen, argon, oxygen, air, helium, hydrogen and methane. This study addresses three of the most common cryogens: nitrogen, argon and oxygen. Hydrogen and helium have very low Prandtl number, and as such they pose more challenges for numerical simulation [7]. By studying the momentum and heat transfer characteristics of nitrogen, oxygen and argon in this work, liquid air which is composed of mainly these three is also covered. The correlations which are derived from the study of these three constituents would also be applicable to liquefied air.

From thermodynamic considerations, the temperature of the interface between liquid and its vapor is assumed to be the saturation temperature of the liquid at atmospheric pressure. The temperature of the pipe is set approximately at the room temperature. The liquid phase does not have any subcooling. The temperature of the interface is the same as saturation temperature of the liquid phase. These sets of assumptions closely resemble realistic conditions in cryogenic chill down.

During the chill down process, rapid heat transfer happens through film boiling, since the temperature difference between the liquid and the wall exceeds the Leidenfrost point. As more liquid enters the pipe, larger surface area will be available for the phase change. Due to this, the velocity of the vapor phase and the mass flow rate will increase continuously. In [7], the case of constant wall temperature was also simulated. However, this is the limiting case for heat transfer when the pipe has an infinite heat capacity and ultimately all of the liquid should get vaporized. This is not what will happen in the real situation. The pipe will be quenched and ultimately come to the same temperature as the
cryogen. Therefore in this research only the case of pipe with finite wall thickness (in other words, finite heat capacity) will be studied.

The pipe material for this study is chosen to be a Titanium alloy, to allow the results to be compared with [7]. The properties of this material are $\rho = 4450 \text{ kg/m}^3$, $C_p = 4200 \text{ J/kg.K}$ and $k = 4.8 \text{ W/m.K}$. The thickness of the pipe is chosen to be $\Delta R = R_{wo} - R_{wi} = 0.02R$. The non-dimensional parameters in this study are the Reynolds number, the Jakob number, the Peclet number and the Weber number. The ratio of fluid properties also plays a role. It is to be noted that the definition of $Ja$ is different from [7] in this study, and corresponds to the standard definition given in [10]. For example $Ja = 1630$ is chosen for all the cases of $N_2$ chill down. This corresponds to the case with $Ja = 0.42$ in [7]. See Eq. 3–17 for the definition of these parameters. The effects of these parameters have been studied in more detail than [7]. Also, in the present study the simulations are done for a much longer time and therefore give more insight into the physics of cryogenic chill down.

6.2 Cryogenic Chill Down of Nitrogen

Liquid nitrogen is an important cryogen with many applications in space missions. It has been studied by [7] in detail. In our research, only a few cases of $N_2$ will be studied and they will be compared with [7]. The values of the non-dimensional parameters for these cases are listed in the Table 6-1 for easy reference. The parameters are chosen to match the values in the study by [7].

The properties of $N_2$ are taken at 300 $K$ and 77 $K$ under 1 atm. Therefore the ratio of fluid properties is constant for $N_2$ study. The inlet velocity of the liquid and vapor phase is also constant in these computations and set to be 10$cm/s$. In this study, the role of the Reynolds number on heat transfer characteristics and phase change has been studied. Four cases have been studied: $Re = 1000$, $Re = 1500$, $Re = 2043$ and $Re = 3000$. The value of $Re = 2043$ was chosen to compare the results with [7]. It is to be noted that even though the $Re = 3000$, the flow has been assumed to be laminar. This
assumption can be justified because research suggests that for smooth entry the transition from laminar to turbulence can be delayed significantly. The critical Reynolds number in pipe flow may increase by 60% from the value of 2300 which is usually taken [88, 89]. The Peclet number cannot be changed independently, and it becomes determined once the Reynolds number and the liquid is chosen. The pipe diameter corresponding to $Re = 2043$ case is $4mm$. The thickness of the pipe is chosen to be $\Delta R = R_{wo} - R_{wi} = 0.02R$. In the present cases, radiation effects have not been included.

Table 6-1. Parameters for $N_2$ chill down simulation

<table>
<thead>
<tr>
<th>Case</th>
<th>$Re$</th>
<th>$Ja$</th>
<th>$Pe$</th>
<th>$We$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>1000</td>
<td>1630</td>
<td>2320</td>
<td>1.84</td>
</tr>
<tr>
<td>Case 2</td>
<td>1500</td>
<td>1630</td>
<td>3480</td>
<td>2.77</td>
</tr>
<tr>
<td>Case 3</td>
<td>2043</td>
<td>1630</td>
<td>4739</td>
<td>3.69</td>
</tr>
<tr>
<td>Case 4</td>
<td>3000</td>
<td>1630</td>
<td>6960</td>
<td>5.53</td>
</tr>
</tbody>
</table>

Figures 6-1, 6-2 and 6-3 show the contours of $U$ and $V$ components of velocity and the temperature at time $t = 0.4$ for Case 3. This results from [7] are showed alongside for comparison which use the same $Re, Pe, We$ and $Pe$. The flow patterns look almost identical. It is seen that the maximum in $U$ and $V$ is very close to that obtained by [7], with the present simulations producing slightly lower velocities. This is because in the present case, the effects of radiation from the wall have not been included, whereas they have been modeled in [7].

Next, results of $U$ and $V$ velocity components and temperature for the four cases with different Reynolds number are presented in Figures 6-4, 6-5 and 6-6. Except for the case $Re = 2043$, the other cases have only been studied by [7] for the constant wall temperature case. These results highlight the fact that maximum phase change takes place in the
Figure 6-1. U-velocity contours of Liq. $N_2$ at $t=0.4$ [Reprinted with permission from Tai, C.F. 2008. Cryogenic two-phase flow and phase-change heat transfer in microgravity, PhD Dissertation (Page 162 Figure 7-29). University of Florida, Gainesville, Florida.]

narrow gap between the liquid core and the wall of the pipe. The localized high velocities
occur in the constriction zone where the slight bulge in the liquid front is present. At this location, the mass flow rate is highest, and the area available for it is the most narrow.

Although the basic flow patterns are very similar for all the cases, the maximum values of U and V velocities attained are vastly different. It is seen that an inverse relationship exists between the velocities and the Reynolds number of the flow. This is an expected outcome because the temperature gradients for all the four cases are approximately the same, as can be seen in Figure 6-6. Therefore, from Eq. 3–15, the mass flux generated at the interface is inversely proportional to the Peclet number, i.e.

$$\dot{m}' \propto \frac{Ja}{Pe}$$

(6–1)

Since the Ja is same for all the cases, and $Pe = Pr \cdot Re$, so the rate of mass generation should vary inversely as $Re$.

Figure 6-7 shows the temperature at the inner wall of the pipe for $Re = 1000$ and $Re = 2043$ at three different time instants. Here the wall chill down effect can be clearly
Figure 6-4. U-velocity contours of Liq. $N_2$ at $t = 1.5$ for different $Re$

seen. They show good match with the results of [7]. As the liquid enters the pipe, more
and more cooling takes place. Since the liquid is at saturation temperature, so the heat
transfer from the pipe wall to the liquid causes evaporation at the interface. The rate
of heat transfer different for the two cases seen in Figure 6-7A and 6-7B. However, a
direct comparison is not valuable here because both $Re$ and $We$ are different for the two
cases. The effect seen here is therefore the combined effect of the two parameters. For this
Figure 6-5. V-velocity contours of Liq. $N_2$ at $t = 1.5$ for different Re

reason, later their effect will be investigated separately by varying only one of them at a time.

Figure 6-8 shows the non-dimensional mass flow rate at the pipe exit for the four cases as a function of time. The flow rate constantly increases during the chill down, as more and more liquid enters the pipe. It can be clearly seen that the rate of evaporation is influenced by the Re of the flow. To investigate this effect further, the mass flow at $t = 1.5$
Figure 6-6. Temperature contours of Liq. $N_2$ at $t = 1.5$ for different $Re$

is taken and plotted as a function of $Re$ in Figure 6-9. In this figure, it is clear that the heat transfer is inversely proportional to the $Re$ of the flow.

### 6.3 Cryogenic Chill Down of Oxygen

Liquid oxygen is another important cryogen with many applications. Therefore in this research liquid oxygen chill down is studied in depth to examine the effect of various physical parameters, viz. $Re$, $We$ and $Ja$. The Peclet number cannot be varied independently of the Reynolds number since $Pe = Pr \cdot Re$ and $Pr$ depends only on the
Figure 6-7. Temperature at $r = R_i$ for Liq. $N_2$

Figure 6-8. Non-dimensional mass flow rate history for $N_2$

liquid properties. The diameter, velocity and initial wall temperature are changed to keep the rest of the non-dimensional parameters constant while varying only the parameter of interest. The velocity and diameter determine the $Re$ and $We$ while the wall temperature decides the $Ja$. Radiation effects are included in the computations. The wall temperature varies during the computations, as the wall gets cooled down by heat transfer to the liquid
Figure 6-9. Non-dimensional mass flow rate at $t = 1.5$ for $N_2$

phase. Rapid evaporation takes place from the liquid-vapor interface via film boiling. A recirculation zone soon develops near the liquid front, leading to higher mixing and heat transfer.

Figure 6-10 shows the typical flow patterns observed for $O_2$ in the simulations performed in our study. The case selected is Case 1 from Table 6-2 with $Re = 3000$. After the implementation of the QUICK scheme, the simulations can be performed even when $Pe >> 2$. This figure shows the velocity and temperature contours. The interface shows a bulge near the tip due to the effect of surface tension. The distance between the interface and the wall is relatively constant for a long section. The velocity of the liquid slug is nearly constant throughout. The velocity of the vapor phase shows a lot of variation in the flow. At the inlet, the vapor starts with a velocity equal to that of the liquid phase. Due to the strong temperature gradient set up in the narrow space between the interface and the wall, film boiling takes place. Since the liquid is not subcooled, so all the heat transferred to the interface from the wall (via convection and radiation) is used up for phase change. This causes a steady increase in the vapor velocity as we travel along the $x$-direction. Near the tip of the interface the velocity of the vapor phase
Figure 6-10. Flow field of $O_2$ at $t = 8.0$ for Re=3000

is maximum. This is partly due to the bulge in the interface, which accelerates the vapor further. The tip of the interface is located at approximately $x = 8.3$ at $t = 8.0$ for the case shown. The very high vapor velocity near the tip, and the subsequent diffusion into a much wider space, gives an effect similar to the flow over a (smooth) backward facing step. There is a vortex formed at the liquid front when the vapor velocity becomes higher. The negative $U$-velocities in this zone are due to the recirculation. This can also be seen in the $V$-velocity plot, Figure 6-10B. The velocity changes from positive to negative in the space
in front of the liquid slug. The temperature contours can be seen in Figure 6-10C. It can be seen that the wall is significantly chilled down near the entrance of the pipe.

![Temperature Contours](image)

Figure 6-11. Development of the flow field for a typical case of $O_2$

Figure 6-11 shows snapshots of the flow field at different time instants. It can be seen that there is no vortex at $t = 2.0$, it is starting to develop at $t = 5.0$ and grows bigger in size by $t = 8.0$. This is because at $t = 2.0$ the vapor velocity is not high enough. As it increases further, a vortex starts developing. Due to the presence of the recirculation zone, more mixing can take place at the liquid front with enhanced heat transfer. Figure 6-12 shows the temperature contours for the same case at $t = 8.0$, in which it is clear that the vapor phase is significantly cooler near the liquid front due to the presence of the vortex.

Figure 6-13 shows the pressure at the centerline ($y = 0.0$) and the wall ($y = 0.5$) at $t = 8.0$ for the same case. The pressure at the center line is actually the pressure of the liquid phase in the two-phase region (up to about $x = 8.3$). The pressure at the wall corresponds to the pressure of the vapor phase. It can be seen that the pressure gradient is not constant in the two-phase region. This is expected, because the mass flow rate of
Figure 6-12. Temperature contours near the liquid front, $Re = 3000$

Figure 6-13. Pressure at center line and wall for $O_2$, $t = 8.0$, $Re = 3000$

vapor is continuously increasing up to about $x = 8.3$. The $x$-gradient of vapor velocity is positive which gives a negative pressure gradient which becomes steeper with $x$. The pressure in the liquid phase is related to the pressure in the vapor phase by the interfacial normal stress balance. The difference between the two is due to the effect of surface tension and the relatively small normal stresses at the interface. There is a sharp peak in the pressure of the liquid near the tip of the interface because of the high curvature and
the consequent strong surface tension. Beyond $x = 8.3$, the two lines merge into one. This is because in single-phase pipe flow, the $y$-gradient of pressure is negligibly small. The pressure gradient settles down to a small negative but constant value in the single phase region as expected.

Figure 6-14. Time dependence of wall temperature for $O_2$, $Re = 3000$

Figure 6-14 shows the temperature of the solid-gas interface as a function of time. Initially, the wall starts out at a uniform non-dimensional temperature of $T = 1.0$. At $t = 2.0$, the interface is located at approximately $x = 2.4$ as can be seen in Figure 6-11. It is seen that significant cooling of the wall has occurred up to about $x = 2.4$, but beyond that region the temperature of the wall is still close to the initial value. As the interface advances further, more and more of the wall chills down. Significant cooling takes place in the two-phase region, but as time increases, the rest of the wall also sees some cooling effect. At $t = 5.0$, even though the interface is located at $x = 5.3$, the wall temperature up to $x = 10.0$ has started to decrease. This is due to the cooler vapor evaporating from the liquid surface and traveling downstream.

Figure 6-15 shows how the temperature gradient at the wall changes with time. For the purpose of analysis, the figure can be divided into three sections. In the initial
Figure 6-15. Temperature gradient at wall for $O_2$, $Re = 3000$

section where the temperature gradient is high is the two-phase region. After this comes the transition zone where the gradient first peaks and then there is a sharp drop as the flow transitions into single phase. In the third section, the flow consists of only the vapor phase and the gradients are much lower. Very close to the inlet, the temperature gradient is extremely high due to entrance effect and should be ignored. The temperature gradient drops very quickly and reaches a value around 8.0 for $t = 2.0$ case. In the second part of the curve, there is a peak in the gradient near the tip of the interface. This is because of the deformation of the interface by surface tension, which brings it closer to the wall causing a bulge. The gradient drops after this as the distance of the interface from the wall increases sharply and becomes zero at the tip. In the single phase region, the gradient is much lower. It is interesting to note how the gradient changes with time. For $t = 2.0$ case, the gradient is higher in the initial two-phase region than the other two time instants. This is because the wall temperature is much higher initially. As the wall chills down with time, the gradient becomes lower in this section. In the single-phase region, the trend is opposite. The gradient is much lower at $t = 2.0$ than at $t = 4.0$ or $t = 8.0$. This can be explained by the fact that the vapor phase is getting cooled down in
the single phase region. This increases the temperature difference between the wall and vapor, thus causing the temperature gradient rise with time. In the middle section where a maxima occurs, the gradient first increases with time and then decreases. This can be explained as follows. The gradient depends both on the temperature difference as well as the distance. Initially, the deformation of the interface increases, bringing it closer to the wall. Therefore at $t = 4.0$, the peak is maximum. This leads to enhanced heat transfer to this section of the interface and evaporation to this part of the interface. The gap between the interface and the wall again increases as more and more phase change takes place from this localized area. At the same time, the wall temperature starts to come down, as seen in Figure 6-14. This combined effect reduces the maximum temperature gradient observed at $t = 8.0$.

Figure 6-16. Time dependence of mass flow at pipe exit, $O_2$, $Re = 3000$

Figure 6-16 shows the vapor mass flow rate at the pipe exit. The flow rate presented is non-dimensional. It is seen that the quantity of vapor exiting the pipe is almost linearly increasing with time. The film boiling from the liquid surface feeds into the vapor mass. As more and more surface area is available, the rate of phase change would increase. There is a slight non-linear effect detected at the end of the simulation near $t = 8.0$ with
slowing down of the rate of increase mass flow. This is due to the cooling down of the wall by the cryogen.

6.3.1 Effect of Reynolds Number

Reynolds number is an important factor which affects the convective heat transfer from the pipe wall. It has been shown in the study with liquid $N_2$, that it directly affects the rate of evaporation from the liquid surface. Here, a more detailed study will be undertaken to see the role of $Re$ in oxygen chill down. For this purpose, three test cases are chosen. In this set of cases shown in Table 6-2, only the $Re$ (and $Pe$) is changed. The initial wall temperature for all three cases is 300 K.

To understand the role of the $Re$, we need to see what is happening at the interface. Combining Eq. 3–13 and 3–15 gives

$$\dot{m}'' = \frac{\rho_v J_a}{Pe} \left( \frac{k_v}{k_l} \frac{\partial T_v}{\partial n} - \frac{\partial T_l}{\partial n} + \frac{\dot{q}_i''}{k_l \Delta T} \right) \quad (6–2)$$

In the non-dimensional problem studied here, the temperature gradient is the approximately same for all the cases, provided the interface deformation is not very different. Since the $We$ is same for all the cases, it is expected that the interface shape is going to be similar. Since liquid temperature is constant, the factors affecting the phase change are $Ja$, $Pe$ and vapor and liquid properties. Radiation also plays some role.

Figure 6-18 shows the mass flow rate at $t = 8.0$ as a function of $Re$. The mass flow rate is an indicator of the evaporation taking place at the interface. The trend is similar to that observed with $N_2$ and it is seen that the non-dimensional rate of evaporation is inversely proportional to $Re$.

Figure 6-17 shows the wall temperature at $t = 8.0$ for the three cases. The $Re$ does not have a significant influence on the wall cooling. Lower Reynolds number produces more wall cooling, but the difference between the three temperature profiles is not big. This can be explained by the fact that the flow is assumed to be laminar. In laminar flow, the $Nu$ does not depend on $Re$. This can be seen more clearly in Figure 6-19.
Table 6-2. Parameters for $O_2$ Reynolds number study

<table>
<thead>
<tr>
<th>Case</th>
<th>Diameter (m)</th>
<th>Velocity (m/s)</th>
<th>Re</th>
<th>We</th>
<th>Ja</th>
<th>Pe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.0100</td>
<td>5.15E-2</td>
<td>3000</td>
<td>2.29</td>
<td>1468</td>
<td>6585</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.0069</td>
<td>6.18E-2</td>
<td>2500</td>
<td>2.29</td>
<td>1468</td>
<td>5487</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.0044</td>
<td>7.72E-2</td>
<td>2000</td>
<td>2.29</td>
<td>1468</td>
<td>4390</td>
</tr>
</tbody>
</table>

Figure 6-17. Dependence of wall temperature on $Re$ for $O_2$ at $t = 8.0$

In Figure 6-19B, it can be seen that at $t = 8.0$, the Nusselt number for all the three cases is very close. Here the $Nu_1$ number is defined as

$$Nu_1 = \frac{q''_{w-v} D}{T_w - T_v k_v}$$

where $q''_{w-v}$ is the flux from the wall to vapor phase, $T_w$ is the temperature of the wall and $T_v$ is the mixing cup or bulk temperature of the vapor phase defined by [90]. Although $Re$ has an effect on the temperature gradient, it does not affect $Nu_1$. This is because the reference temperature is now the bulk temperature of the vapor phase $T_v$. As the vapor
Figure 6-18. Non-dimensional mass flow rate at $t = 8.0$ for $O_2$

phase gets cooled down, the temperature gradient drops, but along with it the driving temperature difference $T_w - T_v$ also decreases. Therefore $Nu_1$ remains constant. For the same reason, in Figure 6-19A, in the single phase region (after about $x = 8.3$) the gradient is continuously decreasing. However, in Figure 6-19B $Nu_1$ approaches the value of $3.657$ calculated for single phase laminar pipe flow with constant wall temperature. As already seen in Figure 6-17, the cooling effect far from the interface is small and the pipe wall is still close to the initial temperature, mimicking a constant temperature wall. The two-phase flow enhances the heat transfer with $Nu_1 \geq 16$, which is a very large increase. $Nu_1$ reaches almost the value of 19 near the liquid front because the distance between the wall and the interface is lesser.

6.3.2 Effect of Weber Number

The $We$ also affects the heat transfer in the cryogenic chilldown process. This is because surface tension affects the curvature of the interface near the liquid front. A higher surface tension is expected to cause a greater bulge as shown by [7]. This brings the interface closer to the hot pipe wall and enhances the heat transfer and rate of evaporation.
Figure 6-19. Temperature gradient and $Nu_1$ at $t = 8.0$ for $O_2$ at the interface. Three different cases of $We$ are studied, keeping $Re$, $Pe$ and $Ja$ constant. These are listed in Table 6-3. The wall temperature is 300 K for all the three cases.

Table 6-3. Parameters for $O_2$ Weber number study

<table>
<thead>
<tr>
<th>Diameter (m)</th>
<th>Velocity (m/s)</th>
<th>Re</th>
<th>We</th>
<th>Ja</th>
<th>Pe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.005</td>
<td>8.58E-2</td>
<td>2500</td>
<td>3.19</td>
<td>1468</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.01</td>
<td>4.29E-2</td>
<td>2500</td>
<td>1.59</td>
<td>1468</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.05</td>
<td>8.58E-3</td>
<td>2500</td>
<td>0.319</td>
<td>1468</td>
</tr>
</tbody>
</table>

Figure 6-20 shows the interface shapes at time $t = 2.0$. The lowest $We$ (highest surface tension) case has the greatest deformation near the liquid front. Since the liquid has not spent enough time inside the pipe for significant evaporation to take place, the change in shape can be attributed almost entirely to the surface tension force. It can also be observed that due to conservation of mass and constant liquid influx, the location of
Interface tip is different for the three cases. The temperature gradient of the gas phase would be higher in the region near the bulge, and it is expected to produce a higher local rate of evaporation. The velocity field around the front is also affected, with higher local velocity occurring for the lowest We. Figure 6-21 shows the velocity field for the two extreme cases.

Figure 6-20. Interface shape for different We at $t = 2.0$

Figure 6-21. U-velocity profile of $O_2$ for different We at $t = 2.0$
Figure 6-22. Heat transfer for different We at t = 2.0

Figure 6-23. Heat transfer characteristics for different We at t = 8.0

Figure 6-22A shows the temperature gradient at the interface at the same time instant. The number of marker points is different for the two cases because of the different interfacial length. The peak in the gradient occurs at the position where the local curvature is high due to surface tension. Temperature gradient is much higher for
the lower $We$ case as expected. This is due to the relative proximity of the interface to the wall. The local oscillations are due to the velocity field and interface shape. In Figure 6-22B it can be seen that the cooling effect is much more due to lower $We$ and higher deformation of the interface.

In Figure 6-23, the temperature gradient and Nusselt number for two $We$ are plotted. The case of $We = 0.319$ becomes unstable before $t = 8.0$ is reached. Therefore, its results are excluded from this set of figures. It is seen that the $We$ affects the Nusselt number only locally near the liquid front. In this case too, it is the distance of the interface from the wall which is the controlling mechanism in increasing the temperature gradient and $Nu_1$. Therefore, it can be concluded that $We$ plays an important role by enhancing the local heat transfer near the liquid front.

### 6.3.3 Effect of Jakob Number

The $Ja$ is expected to have a substantial effect on the heat transfer in phase change flows. Eq. 6–2 shows the role of $Ja$ on the evaporation rate. In cryogenic chill down flows, $Ja$ is very high. To study the influence of $Ja$ on heat transfer, the degree of wall superheat has been varied. The baseline case has 300 $K$ as the initial wall temperature, and is the same as Case 2 in the $We$ number study. The other two cases have the same $Re$, $Pe$ and $We$. The diameter is 1 $cm$ and the velocity is 4.29 $cm/s$ for all the cases. They are listed in Table 6-4. It is to be noted that the properties of the gas phase are different for these three cases. Figure 6-24 shows the interface shapes for the three cases at $t = 8.0$. Since the $We$ is constant, the shape change here is almost completely due to phase change at the interface. It can be seen that the case with the highest $Ja$ has the flattest interface shape.

Figure 6-25 shows the mass flow rates at the pipe exit as function of time for all the three cases. The trend agrees with the prediction from theory. The mass flow rate is directly proportional to the $Ja$. The non-dimensional mass flow rate increases linearly with time. Figure 6-26 shows the wall cooling as a function of $Ja$. It is interesting to note
Table 6-4. Parameters for $O_2$ Jakob number study

<table>
<thead>
<tr>
<th>Case</th>
<th>Wall Temperature (K)</th>
<th>Re</th>
<th>We</th>
<th>Ja</th>
<th>Pe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>250</td>
<td>2500</td>
<td>1.59</td>
<td>931</td>
<td>5487</td>
</tr>
<tr>
<td>Case 2</td>
<td>300</td>
<td>2500</td>
<td>1.59</td>
<td>1468</td>
<td>5487</td>
</tr>
<tr>
<td>Case 3</td>
<td>250</td>
<td>2500</td>
<td>1.59</td>
<td>2122</td>
<td>5487</td>
</tr>
</tbody>
</table>

Figure 6-24. Interface shape for different $Ja$ at $t = 8.0$

that $Ja$ has a much more pronounced effect on the wall chill down, as compared to $Re$.
Both the $Ja$ and $Re$ influence the mass flow rate, but their influence on wall chill down is disparate.

To study the effect on heat transfer characteristics further, the temperature gradient and $Nu_1$ are shown in Figure 6-27. For the purpose of analysis, the graphs can be divided into three distinct sections: the initial section of the curve, which corresponds to the section of the interface almost parallel to the wall and with no significant deformation; the middle section where there is a sharp change in the gradient which corresponds to the
curved liquid front; and the final section where there is gradients are much lower because it represents the single phase flow regime. In Figure 6-27A, for the first section of the curve, the gradient is about the same for all the three cases. This is because the distance of the interface from the wall is similar. However, the Nusselt number $Nu_1$ is different in the same section of the curve. This is because the driving temperature difference $T_w - T_v$ is different for the three cases. For example, wall temperature for $Ja = 2122$ is much lower.
Figure 6-27. Heat transfer characteristics for different $Ja$ at $t = 8.0$

than for $Ja = 931$. If the mean temperature of the vapor is similar, then this would give a higher $Nu_1$ for the higher $Ja$.

In the second section of the curves, i.e., near the maxima or peak, $Nu_1$ trend is reversed. This is primarily due to the different shape of the interface for the three cases, as can be noted in Figure 6-24. The interface shape is controlled by the rate of evaporation, which is directly proportional to $Ja$. The flatter profile for higher $Ja$ in this region at $t = 8.0$ gives a relatively lower Nusselt number. Another feature to be noted is that the curve for $Ja = 1468$ has a decidedly higher maxima that Case 2 of the Reynolds number study. This difference can be attributed to the lower $We$ in the Jakob number study.

In the third section of the curves, where the sharp drop occurs at the liquid front and the flow transitions to single-phase, Nusselt number for $Ja = 2122$ is highest. This is because more volume of the newly generated colder vapor is available to chill down the wall by heat transfer. However, all three curves approach the single-phase constant temperature flow value asymptotically.
Figure 6-28. Flow field of Ar at $t = 8.0$ for Re=2500

6.4 Cryogenic Chill Down of Argon

In this section, the results for chill down of argon are presented. This study is organized in a similar fashion to oxygen. For this set of results, most of the non-dimensional parameters have been kept the same as for oxygen. The fluid properties being different, only the parameters like $Pe$ and fluid property ratios are different. Therefore, a direct comparison between argon and oxygen can provide insights about the role of fluid properties in chill down flows. The exact values of the parameters are listed in Tables 6-5,
6-6 and 6-7. For the \( We \) and \( Re \) study, the initial wall temperature is 319 K. For the \( Ja \) study, the velocity is 2.95 \( cm \) and the diameter is 1.64 \( cm \) while the initial wall temperature is different for each case. Radiation effects are included in the computations. The wall temperature varies during the simulations, as the wall gets cooled down by film boiling from the liquid phase.

Figure 6-28 shows the velocity field for a typical case of Argon. The interface shape and the general features of the flow are similar to those found with Oxygen in Figure 6-10. Here too, a vortex is seen at the liquid front. The interface shows the characteristic bulging near the end. The maximum vapor velocity occurs in the region between this swell and the wall. The recirculation zone is formed at the tip of the liquid and can be seen by the negative U-velocity in Figure 6-28A. In the V-velocity plot it can be located by the closely spaced regions of high positive and negative V-velocities formed due to the swirling of vapor. The temperature plot shows a larger boundary layer at the leading edge of the liquid phase due to the mixing of cold and hot vapor in this region.

Figure 6-29. Development of the flow field for a typical case.
6.4.1 Effect of Reynolds Number

In this section, the role of Reynolds number in the cryogenic chill down of Argon is investigated. The parameters are listed in Table 6-5. The general format is similar to that followed with Oxygen. The values or $Re$, $We$ and $Ja$ have been matched with Oxygen, only the $Pe$ being different. So in addition to $Re$, the influence of $Pe$ on flow characteristics will also be studied.

Table 6-5. Parameters for argon Reynolds number study

<table>
<thead>
<tr>
<th>Case</th>
<th>Diameter (m)</th>
<th>Velocity (m/s)</th>
<th>Re</th>
<th>We</th>
<th>Ja</th>
<th>Pe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.0164</td>
<td>3.54E-2</td>
<td>3000</td>
<td>2.29</td>
<td>1468</td>
<td>7221</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.0114</td>
<td>4.25E-2</td>
<td>2500</td>
<td>2.29</td>
<td>1468</td>
<td>6018</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.0073</td>
<td>5.31E-2</td>
<td>2000</td>
<td>2.29</td>
<td>1468</td>
<td>4814</td>
</tr>
</tbody>
</table>

The non-dimensionalized mass flow rate at pipe exit at $t = 8.0$ is shown in Figure 6-31. The flow rate is inversely proportional to the $Re$, but is lower than that
Figure 6-31. Comparison of mass flow rate for Ar and O2 of oxygen for the same Reynolds number. This difference between the two gases is due to the effect of the $Pe$ as demonstrated in Eq. 6-2. Figure 6-32A shows the wall temperature for the three $Re$. The temperatures show a similar trend to Figure 6-17 with respect to the Reynolds number. The wall chill down effect is more for lower Reynolds number.

Figure 6-32. Dependence of wall temperature on $Re$ for Ar at $t = 8.0$
Figure 6-33. Heat transfer at wall for Ar, \( t = 8.0 \)

Figure 6-33 compares the heat transfer characteristics of oxygen and argon. In Figure 6-32B, the wall cooling for oxygen is significantly more. It shows that for the same \( Re \), \( We \) and \( Ja \), oxygen is a more effective coolant than argon due to its fluid properties. The Nusselt number \( Nu_1 \) is plotted in Figure 6-33B for the same case. \( Nu_1 \) for the two fluids is about the same. This is because Nusselt number depends on the temperature gradient, \( T_w \) and \( T_v \). As long as the ratio of the temperature gradient and the driving temperature difference \( T_w - T_v \) is the same, \( Nu_1 \) is not affected.

6.4.2 Effect of Weber Number

The Weber number is a measure of the ratio of fluid’s inertia force to its surface tension force. A higher \( We \) implies a lower surface tension, and vice versa. \( We \) controls the deformation of the interface, especially near the tip where curvature is high since the liquid front has a rounded shape. In the cryogenic chill down process, \( We \) affects heat transfer by controlling the deformation of the liquid front. At low \( We \approx O(1) \), a characteristic bulging takes place bringing the interface closer to the hot pipe walls. Figure 6-34 shows the shapes obtained for three different cases at \( t = 1.0 \). The difference
in shape of interfaces can clearly be observed. The set of non-dimensional parameters for this study are described in Table 6-6.

Table 6-6. Parameters for argon Weber number study

<table>
<thead>
<tr>
<th>Case</th>
<th>Diameter (m)</th>
<th>Velocity (m/s)</th>
<th>Re</th>
<th>We</th>
<th>Ja</th>
<th>Pe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>0.0082</td>
<td>5.90E-2</td>
<td>2500</td>
<td>3.19</td>
<td>1468</td>
<td>6018</td>
</tr>
<tr>
<td>Case 2</td>
<td>0.0164</td>
<td>2.95E-2</td>
<td>2500</td>
<td>1.59</td>
<td>1468</td>
<td>6018</td>
</tr>
<tr>
<td>Case 3</td>
<td>0.0822</td>
<td>5.90E-3</td>
<td>2500</td>
<td>0.319</td>
<td>1468</td>
<td>6018</td>
</tr>
</tbody>
</table>

Figure 6-34. Interface shape for different We at \( t = 1.0 \)

6.4.3 Effect of Jakob Number

It was found in the corresponding study on oxygen that \( Ja \) has a measurable effect on the wall chill down characteristics. Its role is investigated further by studying chill down of argon. Table 6-7 lists the parameters for the three cases. Figure 6-35 shows the interface shapes obtained with argon, at \( t = 8.0 \). In this study too, the highest \( Ja \) has the flattest interface profile. This is because of higher rate of phase change at the interface.
Table 6-7. Parameters for argon Jakob number study

<table>
<thead>
<tr>
<th>Case</th>
<th>Wall Temperature (K)</th>
<th>Re</th>
<th>We</th>
<th>Ja</th>
<th>Pe</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>263.6</td>
<td>2500</td>
<td>1.59</td>
<td>931</td>
<td>6018</td>
</tr>
<tr>
<td>Case 2</td>
<td>319.0</td>
<td>2500</td>
<td>1.59</td>
<td>1468</td>
<td>6018</td>
</tr>
<tr>
<td>Case 3</td>
<td>373.4</td>
<td>2500</td>
<td>1.59</td>
<td>2122</td>
<td>6018</td>
</tr>
</tbody>
</table>

Figure 6-36A takes this argument further, and shows that the mass flow rate at the pipe exit is directly proportional to the Ja. This is a direct result of film boiling at the liquid surface. In Figure 6-36B, the mass flow rate is compared with oxygen. As is expected, the mass flow rate of argon is lower.

Figure 6-37A shows the wall cooling effect. The general trend is similar to oxygen. The effect of Pe can be seen in Figure 6-37B. The cooling effect is more for the case of oxygen. The Nusselt number is plotted in Figure 6-38. The case of Ja = 931 is excluded because it becomes unstable before t = 8.0 is reached. The Jakob number does have an effect on Nu₁, unlike Re which only affected the mass flow rate. In this case, it can be clearly observed that Ja influences Nu₁ in a complex way. In the regime of two-phase flow parallel to the wall, Nu₁ is higher for the higher Ja. Near the liquid front, the trend is reversed. This can be seen in Figure 6-38A.

6.5 Conclusion

To summarize, the effect of physical parameters on cryogenic chill down in microgravity for three important cryogens, viz. N₂, O₂ and Ar was investigated. The flow was assumed to be laminar. The nitrogen chill down results were found to be in good agreement with [7]. More extensive study was done for oxygen and argon. The database was chosen in such a way as to vary only one non-dimensional parameter out of Re, Ja and We. The
Figure 6-35. Interface shape for different $Ja$ at $t = 8.0$

Figure 6-36. Mass flow history for different $Ja$ for $Ar$

Figure 6-36. Mass flow history for different $Ja$ for $Ar$

effect of $Pe$ was studied by comparing the results of oxygen and argon. It was found that each of the parameters affects the thermal-fluid characteristics of the flows quantitatively. However qualitatively all the results show an underlying similarity in the flow patterns and heat transfer trends. The results are also in line with expectation from theory and most of the variations and physical effects behind them have been explained. The Reynolds
number was found to affect the mass flow rates, but did not have a significant influence on the wall cooling or the Nusselt number. We affected the interface shape at the leading edge of the liquid slug, also influencing the heat transfer and velocity field there. \(Ja\) affects all three quantities of interest, i.e., mass flow rate, wall cooling and the Nusselt...
number. The Prandtl number is purely a function of fluid properties. It has an adverse effect on heat transfer, i.e., a higher Prandtl number of the liquid decreased the mass flow rate and wall cooling. It does not influence the Nusselt number over the whole two-phase flow regime, but causes some variations locally near the maxima. In general however, all the three cryogens show very similar trends. Therefore it can be extrapolated that it is possible to predict the general flow patterns and heat transfer trends for the laminar chilldown of any cryogen (including air, which is a mixture of mainly $N_2$, $O_2$ and $Ar$) from the information about its $Re$, $We$, $Ja$ and $Pr$. 
Convective flow boiling such as which occurs in tubes and channels, is a very complex physical phenomenon. There are many variables which control the process, viz., mass flow rate, heat flux, gravity etc to name a few. Internal flows with boiling heat transfer can be broadly categorized into two types: those with low heat flux (less than the critical heat flux, or CHF), and those with very high heat flux or post-CHF flows. The latter are also referred to as quenching flows. This division helps in understanding the differences in flow patterns typically observed for these flows. For vertical flows with low heat flux, the flow progresses from single phase liquid, to subcooled and/or saturated boiling, annular film boiling (AFB), and finally to dispersed flow. The vapor quality and void fraction increase as we traverse along the flow direction. In quenching flows, instead of annular film boiling, inverted annular film boiling (IAFB) is observed. This is because of the Leidenfrost effect; due to the very high heat flux film boiling occurs and a layer of vapor separates the liquid core and keeps it from touching the hot walls. The annular flow regime is important because of its similarity with IAFB. Both are separated flows with only the position of the two phases reversed. In horizontal internal flows, the orientation of the pipe/channel also affects the flow patterns. In microgravity, the orientation has no influence on the flow patterns.

Due to the complexity of internal flow boiling, accurate prediction about heat transfer must be based on knowledge about the flow regimes from experimental studies. The focus of the present research is on cryogenic chill down in microgravity, in which IAFB is the most common flow regime [25, 30, 31]. This is because the wall superheat is quite high even with the pipe at room temperature. IAFB flow regime also occurs in vertical quenching flows in the post-dryout region [19]. IAFB in terrestrial gravity has also received attention due to its role in the Loss of Coolant Accident (LOCA) failure of nuclear reactors [14]. Controlled experiments are difficult to conduct because the lower
film boiling heat transfer coefficient means extremely high wall temperatures and can cause damage of the equipment. This chapter takes up some of the prediction models for IAFB and the results from the present research will be compared to them.

### 7.1 Prediction Methods for Inverted Annular Flow

There are various correlations, 1D and 2D models proposed to study IAFB each with its own sets of assumptions and simplifications. It would be instructive to discuss some of them here, especially noting the dependence of heat flux on the various parameters.

The earliest work on two-phase flows used correlations derived assuming homogeneous flow. One such correlation is that by [19]. They use a two-phase Reynolds number defined in terms of the equivalent vapor quality $x_E$ of the two-phase mixture and propose a modified form of the Dittus-Boelter equation for film boiling

$$
q''_{w-v} = 0.023 \frac{k_v}{D} Re^{0.8} Pr^{0.4} (T_w - T_{sat})
$$

(7–1)

Here $Re_2 = Re v \left[ x_E + \frac{\rho_v}{\rho_i} (1 - x_E) \right]$.

IAFB has been studied using two-fluid models which reduce it into a 1D problem. The governing equations are used in their integral forms. They need to use closure relations to specify the conditions at the interface. To find the heat transfer at the wall, most researches use a modified form of the equation given by [90] for flow between two concentric annular cylinders

$$
q''_{w-v} = \frac{k_v Nu_{oo}}{2\delta} \frac{(T_w - T_v)}{1 - \frac{q''_{v-i}}{q''_{w-v}} \theta^*}
$$

(7–2)

$q''_{w-v}$ is the heat flux from wall to vapor, $q''_{v-i}$ is the heat flux from the vapor phase to the interface, $\delta$ is the vapor film thickness, $T_v$ is the mean vapor velocity, $Nu_{oo}$ is the Nusselt number if only outer cylinder is heated, $\theta^*$ is an influence coefficient. If the gap between the cylinders is small as compared to the radius, the flow is approximated by laminar flow between parallel plates and $Nu_{oo} = 5.385$ and $\theta^* = 0.346$. For turbulent flow, $Nu_{oo}$ and $\theta^*$ have to be read off from a table. [17] have used the Kays equation and give the following
expression for heat flux leaving the inner wall based on their model

\[ q''_{w-v} = \frac{k_v N_{u_{oo}}}{2\delta (1 - \theta^*)} \left[ (T_w - T_v) - \theta^* (T_w - T_{sat}) \right] \]  \hspace{1cm} (7–3)

They use \( N_{u_{oo}} = 5.385 \) and \( \theta^* = 0.346 \) for laminar flow and use interpolation from the tabular data of [90] in the turbulent region. [18] have also proposed a two-fluid model with a more complicated relationship which takes into account the effect of \( Re_v \) and \( Pr \). This is because they assume the vapor flow to be turbulent and use the Dittus-Boelter correlation to predict heat transfer.

\[ q''_{w-v} = \frac{k_v N_{u_{oo}}}{2\delta \left( 1 - \frac{T_w - T_{sat}}{T_w - T_v} \theta^*^2 \right)} (T_w - T_v) \]  \hspace{1cm} (7–4)

In their equation, both \( N_{u_{oo}} \) and \( \theta^* \) are functions of \( Re_v \) and \( Pr \). \( Re_v \) itself is a function of the void fraction and the mean vapor velocity. [6] also make use of the Kays equation and follow the analysis of [17] for \( \delta \ll R \), but for \( \delta \sim R \) they use the Colburn correlation to estimate the heat transfer at wall

\[ q''_{w-v} = 0.023 \frac{k_v}{2\delta} Re_v^{0.8} Pr_v^{0.33} (T_w - T_v) \]  \hspace{1cm} (7–5)

In their formula, \( Re_v = \rho_v u_v 2\delta / \mu_v \) and is based on vapor film thickness and the mean vapor velocity. In all these equations, the mean vapor temperature has been used as the reference temperature to calculate the heat transfer at the wall.

[10] develops a 2D separated flow model for IAFB which is similar to and based on the concepts of annular flow in condensation. For low interfacial shear and acceleration pressure gradient, they obtain

\[ h = \left[ \frac{\rho_v (\rho_l - \rho_v) gh''_{lv} k_v^3}{4 (z - z_{CHF}) \mu_v (T_w - T_{sat})} \right]^{1/4} \]  \hspace{1cm} (7–6)

\[ h''_{lv} = h_{lv} \left[ 1 + \left( \frac{3}{8} \right) \frac{C_{pv} (T_w - T_{sat})}{h_{lv}} \right] \]  \hspace{1cm} (7–7)
where $z_{CHF}$ is the location where the critical heat flux occurs. This equation is valid for $z > z_{CHF}$.

### 7.2 Evaluation of Heat Transfer Engineering Correlations for the Simulated Results

In the present research, the radiation effects are small (near the inlet, the radiation flux is less than 5 percent of the total wall flux). Therefore it is valid to specify a heat transfer coefficient based on the convective flow heat transfer definition. Looking at the expression for $q''_{w-v}$ in the correlations given in the previous section, the reference temperature is either $T_{sat}$ or $T_v$. The length scale is usually $2\delta$ or $D$. The Dittus-Boelter correlation is only valid for turbulent flow, while the Kays equation has been modified by various researchers with different expressions for $q''_{v-i}/q''_{w-v}$. Therefore, three different definitions of Nusselt number were selected and analyzed to find which would be able to explain the results from all of the cases in the simplest and most effective way.

![Temperature contours for Re=3000, $O_2$](image)

**Figure 7-1.** Temperature contours for Re=3000, $O_2$

The Figure 7-1 shows temperature contour plot at $t = 8.0$ for $Re_l = 3000$. The interface is located at $x = 8.32$. Although the liquid Reynolds number is constant,
the Reynolds number for vapor phase is varying spatially because the vapor velocity is changing. Therefore, to find the average $Re_v$, the mean vapor velocity has to be found by integrating over the cross-sectional area of vapor phase:

$$u_v = \frac{\int A_v u \, dA_v}{A_v} \quad (7-8)$$

In the downstream direction, the temperature of the vapor phase is also increasing. The mean temperature of the vapor phase $T_v$ is found by a similar equation

$$T_v = \frac{\int A_v uT \, dA_v}{\int A_v u \, dA_v} \quad (7-9)$$

The film thickness $\delta$ is defined as the distance between the interface and the wall. The first definition of $Nu$ used is:

$$Nu_1 = \frac{q''_{w-v} D}{T_w - T_v k_v} \quad (7-10)$$

This is the definition used for all the Nusselt number figures in Chapter 6. In laminar single phase pipe flow, $T_v$ is taken as the reference temperature because it was found that this yielded a simpler expression for $Nu$, by virtue of the fact that the non-dimensional temperature profile remains constant, even though the real temperature changes. This was the rationale behind trying $T_v$, besides the fact that downstream of the liquid plug the flow is single phase pipe flow with almost constant temperature. Therefore $Nu_1$ reduces to the standard definition of $Nu$ in this region.

The second definition used is based on $T_v$ and $2\delta$. This definition is tried because $2\delta$ is the hydraulic diameter. This is reasonable because the heat transfer is affected by the distance of the liquid phase from the wall. Therefore in Figure 7-2 $Nu_1$ is much higher in the interfacial zone, but drops drastically in the single phase region. Since the initial distance between the interface and the wall was arbitrarily chosen in this research, this definition also eliminates any effect that this arbitrary choice has on the Nusselt number.
It makes the analysis more general so that it can be applied to any IAFB flow model, irrespective of film thickness $\delta$.

$$Nu_2 = \frac{q''_{w-v}}{T_w - T_v} \frac{2\delta}{k_v}$$  \hspace{1cm} (7-11)

The third definition of Nusselt number is based on the two-phase correlations assuming homogeneous flow (or alternatively assuming no knowledge of the flow regime), where it is difficult to determine the vapor phase temperature. Because of this difficulty, $T_{sat}$ is chosen as the reference temperature, and diameter $D$ is the length scale.

$$Nu_3 = \frac{q''_{w-v}}{T_w - T_{sat}} \frac{D}{k_v}$$  \hspace{1cm} (7-12)

Figure 7-2 shows the plots of $Nu$ for the case in Figure 7-1 based on these definitions. They are compared the value calculated for single phase pipe flow with constant temperature, i.e., $Nu=3.657$. The interface is present till $x = 8.0$ approximately. Beyond that it is only vapor flow. $Nu_3$ was defined based on $T_w - T_{sat}$ as is the convention for two-phase flows. It can be seen that $Nu_3$ is high in the two-phase zone. It is extremely

![Figure 7-2. Comparison of different definitions of Nusselt number](image-url)
high near the inlet due to entrance effect, but very quickly settles to an almost constant
value. Since the reference temperature is $T_{sat}$, this definition of Nusselt number does not
reduce to the standard definition for pipe flow in the vapor only region. $Nu_1$ takes the
mean temperature $T_v$ as the reference which is higher than $T_{sat}$. Therefore $Nu_1$ is higher
than $Nu_3$. In the vapor only zone $Nu_1$ asymptotically reaches the value for single phase
pipe flow. This is because it is standard for single phase to take $T_v$ as the reference to find
$Nu$.

In the Figure 7-2 it can be seen that $Nu_2$ is close to the value predicted for single
phase laminar flow with constant wall temperature everywhere except near the liquid
front. This can be explained as follows.

$$Nu_2 = Nu_1 \frac{2\delta}{D}$$

The vapor film thickness is defined as $\delta = R_o - R_{int}$. $\delta$ stays nearly constant in the
annulus region. However, near the tip of the interface, $\delta$ increases sharply, while $Nu_1$ is
steadily decreasing. This gives a peak at the interface tip (at $x = 8.32$) where $\delta = R_o$.
Physically, this may be because the vapor flow in this region is not parallel, and there is
a recirculation zone which enhances the heat transfer significantly near the liquid front.
However, the fact that $Nu_2$ is almost constant in the two-phase region (excluding the local
maximum) shows the validity of predicting the heat transfer for inverted annular flow
by the single phase correlations. The vapor flow between the wall and liquid plug can be
approximated as flow in an annulus with different inner and outer wall temperatures. In
the single phase region ($x > 8.32$) both $Nu_1$ and $Nu_2$ are close to 3.657. Therefore the
Nusselt number obtained from the current simulations seems reasonable and according to
what one would expect from theory.

Among these definitions of Nusselt number, $Nu_2$ shows the most promise in terms
of developing a correlation or comparing with other researchers, because of its use of $T_v$
and the hydraulic diameter $2\delta$ as reference. If we leave aside the local peak in $Nu_2$ near
the liquid front, it is almost constant in the two-phase region. Next step is to look at \( Nu_2 \) for all the other simulations. Figure 7-3 shows \( Nu_2 \) for all the cases studied for oxygen.

In this figure, the first case of Reynolds number study is denoted as O2-Re-1, the second case as O2-Re-2 and so on. For the list of parameters corresponding to these cases, refer to Table 6-2, 6-3 and 6-4. The \( y \)-axis has been changed to make the differences between the cases clearer. The Nusselt number values for pipe flow with constant temperature (\( Nu_T = 3.657 \)) and constant heat flux (\( Nu_H = 4.364 \)) are also shown. Since the liquid speed at inlet is constant, and all the cases are plotted at \( t = 8.0 \), the position of the interface tip is approximately the same for all the cases, with minor differences due to the deformation near the tip. The overall trend is the same for all the cases. It is seen that the \( Nu_2 \) from all the cases of \( Re \) and \( We \) study almost overlap in the annulus region. The case O2-Ja-3 which has the highest \( Ja = 2122 \) is a little higher than the rest, and the case O2-Ja-1 with \( Ja = 931 \) is a little smaller than the rest of the cases. So \( Nu_2 \) is affected by the \( Ja \) in the annulus region, but not by \( Re \) and \( We \). O2-Ja-3 has the highest \( Nu_2 \) not only in the annulus region but also near the interface tip and in the region just ahead of

![Figure 7-3. \( Nu_2 \) for all the oxygen cases](image)
Figure 7-4. $Nu_2$ for all oxygen and argon cases

the interface. It does however settle down to the value of 3.657 like all the other cases. Figure 7-4 shows all the $O_2$ and $Ar$ cases in this research. The naming convention for the cases is same as for oxygen. The parameters can be looked up in Table 6-5, 6-6 and 6-7. All the Nusselt numbers fall in a narrow band irrespective of the cryogen, with the highest $Nu_2$ occurring for the cases with the highest $Ja$. In the annulus region (away from the entrance and interface tip), all the results lie between the two limits of $Nu_H$ and $Nu_T$.

Next it was decided to compare $Nu_2$ for the representative case O2-Re-1 with some correlations from literature. Figure 7-5 shows $Nu_2$ plotted alongside the values predicted by [17] and the Colburn equation (Eq. 7–5) which has been used by [6] for $\delta \sim R$.

To calculate the Nusselt number from Eq. 7–3, we take the $T_v$, $T_{sat}$ and $T_w$ from the simulations and use $Nu_{\infty} = 5.385$ and $\theta^* = 0.346$ for laminar flow

$$Nu_{Analytis} = \frac{q''_{w-v} 2\delta}{(T_w - T_v) k_v} = \frac{5.385}{(1 - 0.346^2)} \left[ 1 - 0.346 \frac{(T_w - T_{sat})}{(T_w - T_v)} \right]$$ (7-14)
Figure 7-5. Comparison of Nusselt number with other researchers

Similarly, to calculate Nusselt number from Eq. 7–5

$$Nu_{Colburn} = 0.023Re_v^{0.8}Pr_v^{0.33}$$  \hspace{1cm} (7–15)

In the figure, the Nusselt number for single phase flow in a pipe at constant temperature ($Nu_T = 3.657$) and constant heat flux ($Nu_H = 4.364$) are also shown. In general, the comparison with [17] is very good. Near the entrance region ($x < 1.5$) however there are differences between the results from the numerical simulation and the prediction of [17].

[17] predict a much more smoothly varying $Nu$ whereas in the simulations there is sharp drop in $Nu_2$ near the entrance. In the core annulus region away from the entrance and away from the interface tip, the two results closely match. Taking the average of error for $1.5 < x < 8.0$, the agreement with [17] is within 3 percent. This shows that the formulation used by [17] is a very good fit when the vapor film thickness varies smoothly as in the middle section of the liquid plug. Closer to the liquid front, the interface is deformed and $\delta$ first decreases as we go near the bulge and becomes a minimum, and then it again increases as the tip of the interface is reached. The results from the present
research show that $Nu_2$ is affected by changes in $\delta$ whereas the equation by [17] is not able to capture the effect of sharp changes in $\delta$ on the Nusselt number. At the interface tip ($x = 8.32$), the difference between the two is maximum at 53 percent. It should be noted that Eq. 7–3 was derived assuming an annulus with constant inner and outer radii and fully developed flow. Therefore it should be used with caution wherever the flow is not fully developed, for example near the entrance and where there are sharp changes in $\delta$. Also, the result from [17] is not valid in the region beyond the interface as there is no annulus and only vapor flow there, so these points should be ignored.

Although the Colburn equation is mainly valid for turbulent flow, it was chosen because it can be used over the entire flow regime. It is seen that Colburn equation predicts a much lower value of Nusselt number throughout and the agreement with present results is not close, especially in the annulus region. From [91], the range of application for this equation is $0.7 \leq Pr \leq 160$ and $Re > 4000$. For this case, the Reynolds number of the vapor is much lower; $Re_v = 280$ in the vapor phase near the pipe exit. The discrepancy reduces as the Reynolds number of the vapor flow increases along the $x$-direction. In the single-phase flow regime the results are the same order of magnitude, but the error introduced by using Colburn equation even for fully developed vapor flow where the difference is minimum, would be almost fifty percent.

### 7.3 Conclusion

The results from the simulations performed were analyzed to come up with the simplest and most effective representation of the heat transfer coefficient. The Nusselt number $Nu_2$ defined using the mean vapor temperature $T_v$ and the hydraulic diameter $2\delta$ was found to be the best representation. The results were then plotted in terms of $Nu_2$ for all the cases of oxygen and argon studied, and it was found that they all fall in a narrow band and have the same general trend. In the vapor only region of the flow, $Nu_2$ very soon reaches the value 3.657 for single phase pipe flow with constant temperature walls. There was slight increase or decrease in $Nu_2$ based on whether $Ja$ was high or low.
respectively, but the differences were small. The results were then compared with the prediction from the classic Colburn equation and the formulation by [17]. It was found that the present results match closely with the latter’s prediction (within 3 percent) in the middle section of the interface where the flow is fully developed, away from the entrance and interface tip. The error near the entrance and the liquid front was much higher, so the equation by [17] should be used with caution in these regions. The prediction from Colburn equation which is primarily meant for turbulent flow was the same order of magnitude, but the error introduced by using this equation would be very high.
8.1 Summary

In this research, a numerical method for modeling inverted annular film boiling regime during cryogenic chill down in microgravity has been presented. The numerical method consists of Sharp Interface Cut-Cell Method with several enhancements to address some of the unique challenges faced in the simulation of two-phase internal flows. Thorough verification and validation of the SIMCC method with phase change was done through a series of tests. The results of these tests are given in Chapter 5. A summary of all the test problems performed to date is given in Table 8-1. It has been demonstrated that the SIMCC is accurate and fully capable of simulating two-phase flows with phase change.

Table 8-1. Verification and validation study for SIMCC

<table>
<thead>
<tr>
<th>Test Case</th>
<th>Aspect of code tested</th>
<th>Range of Critical Parameter(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lid driven cavity flow</td>
<td>2d Navier Stokes Solver</td>
<td>$100 \leq Re \leq 4000$</td>
</tr>
<tr>
<td>Flow over solid sphere</td>
<td>Sharp Interface Cut-cell algorithms</td>
<td>$1 \leq Re \leq 100$</td>
</tr>
<tr>
<td>Deformable bubble in gravity</td>
<td>Moving Interface algorithm</td>
<td>$1 \leq Re \leq 100, 1 \leq We \leq 10$</td>
</tr>
<tr>
<td>Liquid plug flow</td>
<td>Internal two-phase flows</td>
<td>$Re = 10, 0.05 \leq Ca \leq 0.25$</td>
</tr>
</tbody>
</table>

However, it should be emphasized here that even though the numerical method developed by the previous researchers like $[7, 54, 59, 64, 66]$ offers many advantages for simulating multiphase flows, the inherent complexities of cryogenic chill down process pose several numerical challenges. Therefore the techniques developed by them are not sufficient to simulate the inverted annular flow problem in depth for more challenging cases. The localized high velocities and steep gradients produced because of the unique
geometry of inverted annular flows lead into numerical convective instability problem. These issues in the simulation of internal flows with phase change have been explained further in Chapter 4. The concerns about numerical stability and slow performance for large flow domains were also discussed.

One of the contributions of the present research is that effective remedies and improvements to address these issues, viz. a full multigrid designed especially for SIMCC, and the upwind differencing using QUICK scheme of [70] for the convective term, have been proposed and implemented. The QUICK scheme was demonstrated to effectively alleviate the stability problems associated with the discretization of the convective term for $Pe_{cell} > 2$. The multigrid method was tested for the pressure-Poisson equation without the cut-cells first. It was shown that the performance with multigrid is improved. Next, a test case with an artificial interface embedded in lid driven square cavity was used to test the accuracy and speed enhancement by using multigrid. It was shown that multigrid shows decreases the computation time by a factor of more than 2.5, while maintaining the same level of accuracy. This is very significant improvement in speed. Thus one of the contributions made by this research is to extend the capability of SIMCC to handle internal two-phase flows with phase change.

The improved and enhanced SIMCC was used to simulate chill down of three important cryogens: nitrogen, oxygen and argon. By studying the momentum and heat transfer characteristics of nitrogen, oxygen and argon in this work, liquid air which is composed of mainly these three is also covered. The nitrogen chill down results were found to be in good agreement with [7]. More extensive study was done for oxygen and argon. The database was chosen in such a way as to vary only one non-dimensional parameter out of $Re$, $Ja$ and $We$. The effect of $Pe$ was studied by comparing the results of oxygen and argon. It was found that each of the parameters affects the thermal-fluid characteristics of the flows quantitatively. However qualitatively all the results show an underlying similarity in the flow patterns and heat transfer trends. Therefore it can be
extrapolated that this research would make it possible to predict the general flow patterns and heat transfer trends for the laminar chill down of any cryogen (including air, which is a mixture of mainly $N_2$, $O_2$ and $Ar$) from the information about its $Re$, $We$, $Ja$ and $Pr$.

The results from the simulations performed were analyzed to come up with the simplest and most effective representation of the heat transfer coefficient. The Nusselt number $Nu_2$ defined using the mean vapor temperature $T_v$ and the hydraulic diameter $2\delta$ was found to be the best representation. The results were then plotted in terms of $Nu_2$ for all the cases of oxygen and argon studied, and it was found that they all fall in a narrow band and have the same general trend. It was found that the present results match closely with the latter’s prediction (within 3 percent) in the middle section of the interface where the flow is fully developed, away from the entrance and interface tip. The determination and validation of engineering heat transfer coefficient for inverted annular film boiling for three cryogens is another major contribution of the present research.

### 8.2 Future Directions

The research on cryogenic chill down flows has many interesting possibilities. Some of them are:

**Variable Properties**

The current simulations use constant properties for the vapor phase. For the vapor phase, properties were evaluated at the initial wall temperature, while the liquid was assumed to be at its saturation temperature with no subcooling. Future work can include the effect of temperature on the vapor properties. This is easy to implement, since in the absence of gravity no natural convection can take place. Therefore the basic governing equations will remain the same, provided the flow is still incompressible.

**Turbulence Effects**

Recent research suggests that for smooth entry the transition from laminar to turbulence can be delayed significantly. The critical Reynolds number in pipe flow may increase by 60% from the value of 2300 which is usually taken [88, 89]. The assumption
of laminarity in the current research limits it to \( Re_L \leq 3000 \). If turbulence modeling is included, much higher \( Re_L \) can be explored.

**Three-Dimensional Model**

A three-dimensional sharp interface model would enable simulation of more general flow situations. Researchers like [52, 92–95] have implemented three-dimensional techniques for interface tracking. However, most of these address isothermal flows. In future, these techniques can be developed to handle more complex flows with phase change.

**Simulation of Low Boiling Cryogens**

Low-boiling cryogens like hydrogen, helium and neon have not been included in the present study as they pose more severe challenges in numerical simulation using the present techniques. The \( Ja \) is much higher for these cryogens if chill down of a pipe at room temperature is simulated. They are also more likely to transition into the turbulent regime earlier. To simulate realistic chill down of these cryogens, adaptive mesh refinement with multigrid acceleration would be required. A turbulence model might also be needed.

**Dispersed Flow Model**

The present research is limited to inverted annular film boiling, where both the phases are separated with no intermixing. In actual flow situations, there are always some liquid droplets entrained in the vapor phase, and some bubbles of vapor present in the liquid. Further, the flow regime itself changes to dispersed flow when the vapor quality is high. The present model can not model more than one interfaces to be present in the fluid flow. If the present technique can be extended to include more than one surfaces, a basic dispersed flow model can be implemented.
REFERENCES


BIOGRAPHICAL SKETCH

Alpana Agarwal was born in the city of Lucknow, India. She went to school at St. Agnes Loreto High School until 1997. Thereafter she attended La Martiniere Girls College. She was admitted to the prestigious Indian Insitute of Technology (IIT), Kanpur in the year 2000. She received her Bachelor in Technology (B.Tech.) in Mechanical Engineering in 2004. She worked at GE Global Research, Bangalore in the materials’ mechanics group for a year before deciding to pursue higher studies. She received the Alumni Fellowship at UF and joined the direct Ph.D program in fall of 2005 with Dr. J.N. Chung as her advisor. Since then she has been engaged in research about computational fluid mechanics and heat transfer for multiphase flows using the moving interface techniques.