I, Bradley J. Romanchuk, hereby submit this original work as part of the requirements for the degree of Master of Science in Mechanical Engineering.

It is entitled:
Computational Modeling of Bubble Growth Dynamics in Nucleate Pool Boiling for Pure Water and Aqueous Surfactant Solutions

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Computational Modeling of Bubble Growth Dynamics in Nucleate Pool Boiling for Pure Water and Aqueous Surfactant Solutions

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ABSTRACT

A computational model has been developed to simulate growth of an isolated vapor bubble during nucleate pool boiling of pure water and aqueous surfactant solutions at saturated conditions on a surface with a constant temperature. The governing equations of mass, momentum, and energy conservation are solved in the liquid and the vapor phases using a finite volume method. The Volume-of-Fluid (VOF) method is employed to capture the deforming liquid-vapor interface. The computational domain includes a microlayer near the liquid-solid-vapor contact line and macro region that contains the vapor bubble and the surrounding liquid. Solution of the governing equations in the microlayer provides source terms for the heat transfer and phase change for the macro region. The computational model was validated by comparing with results available in the literature for pure water.

Simulations of bubble growth from incipience to departure are conducted for pure water and surfactant solutions of sodium dodecyl sulfate (SDS), cetyltrimethylammonium bromide (CTAB), and octylphenol ethoxylate (Triton X-100) at twice the Critical Micelle Concentration (2×CMC). Wall superheats of 4K and 8K are considered and their respective growth cycle characteristics are discussed in detail. The results show that the predicted bubble departing volume and growth rate increases leading to a faster departure time as the wall superheat is increased. The time-dependent surface tension relaxation at the liquid-vapor interface along with increased surface wettability at the liquid-solid interface result in smaller bubbles departing with higher frequency in surfactant solutions compared to boiling in pure water. The dynamic surface tension and surface wettability play an important role in governing bubble growth dynamics in nucleate pool boiling of surfactant solutions.
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NOMENCLATURE

\( A \) \quad \text{Hamaker Constant [N\cdot m]}

\( C_p \) \quad \text{Specific Heat at Constant Pressure [kJ/(kg \cdot K)]}

\( E \) \quad \text{Specific Energy [kJ/kg]}

\( F_\sigma \) \quad \text{Volumetric Surface Tension Force [N/m\(^3\)]}

\( g \) \quad \text{Gravitational Acceleration [m/s\(^2\)]}

\( h_{ev} \) \quad \text{Evaporative Heat Transfer Coefficient [W/(m\(^2\)\cdot K)]}

\( h_{fg} \) \quad \text{Latent Heat of Evaporation [kJ/kg]}

\( k \) \quad \text{Thermal Conductivity [W/(m\cdot K)]}

\( \bar{M} \) \quad \text{Molecular Weight [kg/mol]}

\( m' \) \quad \text{Mass Flow Rate [kg/s]}

\( m'' \) \quad \text{Mass Flux [kg/m\(^2\)]}

\( P \) \quad \text{Pressure [N/m\(^2\)]}

\( Q \) \quad \text{Total Heat Transfer [W]}

\( q'' \) \quad \text{Heat Flux [W/m\(^2\)]}

\( \bar{R} \) \quad \text{Universal Gas Constant [kJ/(mol\cdot K)]}

\( R_b \) \quad \text{Bubble Radius [m]}

\( R_{\text{max}} \) \quad \text{Microlayer Outer Radial Coordinate [m]}

\( R_0 \) \quad \text{Microlayer Inner Radial Coordinate [m]}

\( r \) \quad \text{Radial Coordinate [m]}

\( S_E \) \quad \text{Volumetric Energy Source Term [W/m\(^3\)]}
\( S_m \) Volumetric Mass Source Term \([\text{kg/(m}^3\cdot\text{s})]\)

\( T \) Temperature \([\text{K}]\)

\( t \) Time \([\text{s}]\)

\( t_d \) Departure Time \([\text{s}]\)

\( u \) Radial Velocity \([\text{m/s}]\)

\( v \) Vertical Velocity \([\text{m/s}]\)

\( y \) Vertical Coordinate \([\text{m}]\)

\( V_{\text{liq}} \) Liquid Volume for Source Term \([\text{m}^3]\)

Greek Symbols

\( \alpha \) Volume Fraction

\( \beta \) Evaporation and Condensation Accommodation Coefficient

\( \delta \) Microlayer Thickness \([\text{m}]\)

\( \delta_0 \) Equilibrium Microlayer Thickness \([\text{m}]\)

\( \theta \) Contact Angle \( [^\circ] \)

\( \kappa \) Interfacial Curvature \([1/\text{m}]\)

\( \mu \) Dynamic Viscosity \([\text{kg/(m}\cdot\text{s})]\)

\( \nu \) Kinematic Viscosity \([\text{m}^2/\text{s}]\)

\( \rho \) Density \([\text{kg/m}^3]\)

\( \sigma \) Surface Tension \([\text{N/m}]\)

\( [\alpha_i] \) Difference between the Maximum and Minimum Value of \( \alpha \)

\( \langle \alpha_i \rangle \) Arithmetic Mean of \( \alpha \)

Subscripts
\( eff \)  Effective
\( g \)  Growth Time
\( int \)  Interface
\( L \)  Distance from Cavity Center to Measured Position
\( l \)  Liquid
\( LG \)  Liquid-Gas
\( ml \)  Microlayer
\( m_l \)  Liquid Volumetric Mass Source Term
\( m_v \)  Vapor Volumetric Mass Source Term
\( p \)  Pth Phase
\( ref \)  Reference
\( sat \)  Saturation
\( SG \)  Solid-Gas
\( SL \)  Solid-Liquid
\( tc \)  Transient Conduction
\( v \)  Vapor
\( w \)  Wall
INTRODUCTION

1.1 Background

Boiling is a complex phase change process in which vapor bubbles nucleate, grow, and depart from nucleation sites or cavities on a superheated surface. A vapor bubble nucleates when the liquid surrounding the site becomes superheated raising the vapor pressure enough to exceed the ambient liquid pressure and the pressure due to the surface tension force. This process allows the vapor bubble to grow in the surrounding environment. Numerous system variables influence the nature of the boiling process such as heater geometry and orientation, surface finish for cavity dimensions, wettability, liquid temperature (saturated, superheated, or subcooled), system pressure, flow velocity, and so on. Boiling is divided into two modes based on the liquid velocity. Pool boiling occurs when the bulk fluid velocity is zero while flow boiling occurs when there is a finite bulk fluid velocity. Due to the high heat transfer rates associated with boiling, it is used in a variety of applications in HVAC, power, chemical, and thermal processing industries. Improving component thermal performance can increase efficiency, which can reduce size, weight, and cost.

Boiling at the surface of a body fully submerged in a motionless pool of liquid is referred to as pool boiling. The nature of pool boiling differs based on the conditions at which the boiling process takes place. A typical pool boiling curve is shown in Figure 1 as a plot of heat flux versus excess temperature or wall superheat. The excess temperature or wall superheat is the difference between the wall temperature and the saturated bulk liquid temperature. As the wall superheat increases, the pool boiling curve passes through the four labeled regimes. Schematic
representation of the four regimes for pool boiling on a horizontal surface is illustrated in Figure 2. As the heat input to the surface increases, the first mode of heat transfer occurs via natural convection (Region I), which transfers heat from the heated surface to the bulk liquid. At a certain wall superheat (Point A), vapor bubbles begin to appear on the heated surface at certain cavities or nucleation sites; this point is referred to the onset of nucleate boiling (ONB).

Figure 1 – Typical Pool Boiling Curve [Zhang et al. (2004)]
Figure 2 – Regimes on the Pool Boiling Curve [Wasekar et al. (2001)]
These nucleation sites are often made up of microscopic surface scratches or cracks where the trapped liquid vaporizes first creating the liquid vapor interface where the energy transfers in the form of latent heat from the liquid into the vapor. If the surrounding bulk liquid temperature is at or above the saturation temperature, the vapor bubble will grow to a certain diameter, depart from the nucleation site, and rise toward the liquid free surface.

After inception at the ONB point, the boiling curve enters the nucleate boiling regime. If the wall superheat temperature remains at the low end of the nucleate boiling regime labeled as the isolated bubble section (Region II, A-B), bubbles can grow and detach independently from randomly located active nucleation sites on the heated surface. Increasing the wall superheat temperature corresponds to an increase in the number of active nucleation sites and bubble frequency at each site. Eventually, the active sites become spaced so closely that bubbles from separate sites merge together toward the end of their growth process and are released as one. The vapor bubbles are generated and released rapidly, which forces them to merge in the form of slugs and columns (Region II, B-C).

As the wall superheat temperature increases in the regime of slugs and columns (Region II, B-C), vapor bubbles depart more frequently from their activation sites on the surface. This increase in departure frequency inhibits the ability of the liquid to keep the surface completely wetted resulting in a reduced contact area between the superheated liquid and heated surface. This allows vapor patches to form at the surface creating a dry out region decreasing the slope until the heat flux curve achieves a maximum labeled as the critical/maximum heat flux (CHF) condition (Point C), which sets end of the nucleate boiling region.
Increasing the wall temperature beyond the CHF point, the boiling curve enters the transition boiling regime (Region III, C-D). In this regime, the rate of bubble formation exceeds the rate of bubble departure increasing the number of activation sites on the heated surface. The vapor bubbles begin to merge early in the growth cycle from multiple activation sites to create vapor films at various locations on the heated surface quickly increasing the wall superheat. These vapor films are generally unstable and can detach from the surface allowing the surface to become rewetted leading to rapid fluctuations in the surface temperature. Due to the unstable conditions in the transition boiling regime, the wall superheat is taken as an average value. The wall superheat approaches a high enough temperature that the film of vapor becomes steady and the heat flux decreases to a minimum value in the transition boiling region, which is referred to as the Leidenfrost temperature (Point D).

At wall superheats exceeding the Leidenfrost temperature, a fully developed vapor layer entirely splits the bulk liquid and the heated wall, which is known as film boiling (Region IV, D-E). In this section, the phase change process takes place at the liquid-vapor interface as opposed to the heated surface in other regions. The slope of the boiling curve increases in the film boiling regime due to thermal energy from the heated surface traversing through the vapor film. The surface temperature can continue to increase until it reaches the maximum allowable temperature of the material used as the heating surface.

The boiling curve in Figure 1 can be outlined if the surface temperature is controlled and slowly increased. If the surface is heated to the film boiling regime, the pool boiling curve progresses in the reverse order through each regime as the temperature is slowly decreased; however, the path may differ in the transition regime and at the point where nucleate boiling and natural convection meet. The pool boiling curve for a horizontal wall that has a uniform and
controlled heat flux produces a different path than the temperature controlled case shown in Figure 1. When the heat flux is increased to surpass the CHF point, the wall temperature rises to match a higher temperature on the boiling curve skipping over a portion of the nucleate boiling regime and the transition boiling regime. The temperature increase associated with the shift from nucleate boiling to film boiling on an electric heated surface is often large enough to burn out the heater labeling this critical point as the burnout heat flux. If the jump to film boiling is successful and the heat flux continues to increase, the path of the pool boiling curve would follow the film boiling regime in Figure 1.

### 1.2 Scope of Study

Many industrial applications tend to operate in the nucleate boiling regime due to high heat fluxes that correspond to relatively low excess temperatures drawing much research attention. The first section of the present study is to computationally model the growth dynamics of a vapor bubble from incipience to departure in pure water using a constant wall temperature by applying the effects of microlayer evaporation in the micro region and phase change due to the heat transfer from the superheated liquid layer close to the wall in the macro region. An illustration of the two regions is displayed in Figure 3. The heat transfer and phase change in the microlayer near the contact line is determined. For model validation, the results of microlayer shape and heat transfer rate are compared with those available in the literature. The second section introduces surfactant solutions to further understand the effects that dynamic surface tension and surface wettability play in bubble growth dynamics during nucleate pool boiling. Multiple wall superheats are investigated for pure water and surfactant solutions. Their
respective growth rates, vapor profiles, and bubble departure diameter are compared and discussed in detail.

Figure 3 – Macro Region and Microlayer
LITERATURE REVIEW

2.1 Microlayer Development

In order to understand the high heat transfer rates associated with nucleate boiling, a mass transfer mechanism for nucleate boiling referred to as the microlayer theory was proposed by Snyder et al. (1956). They postulated the existence of a thin, viscous liquid layer trapped underneath the vapor bubble on the superheated surface that would continuously evaporate promoting bubble growth as shown in the micro region of Figure 3. Moore et al. (1961) measured the surface temperature during nucleate boiling of saturated water using a single customized fast responsive thermocouple that was flush mounted on the heated surface. During nucleate boiling, the surface temperature fluctuated with time where it would decrease rapidly and then return to its original level; this was the first indirect evidence of a thin liquid film. The microlayer thickness was estimated on the order of 2µm by applying an energy balance for the heat removed during the surface temperature drop. Rogers et al. (1964) extended the work of Moore et al. (1961) by correlating the surface temperature measurements with the bubble growth profiles. A rapid temperature drop was observed as the bubble base advanced over the thermocouple and a temperature recovery when the bubble receded back just prior to departure. The rapid evaporation of the microlayer proved to promote bubble growth, and the recovery temperature permitted the formation of a new microlayer for the next bubble.

Laser interferometry combined with high speed photography was introduced by Sharp et al. (1964) to capture the first direct evidence of the thin liquid film. Reflections from the microlayer were observed through the top of a flattened steam bubble trapped in-between the viewing window and heated surface. A small dry spot formed in the center of the bubble where
its radius expanded as the bubble continued to grow and then disappeared moments after the bubble departed. A wedge like microlayer profile was founded with a thickness of 0.4µm at a bubble radius of 0.94mm. Due to the abnormal conditions of the viewing window constraining the bubble growth, Jawurek et al. (1969) electrically heated a thin transparent film of tin oxide (SnO$_2$) in order to boil methanol and ethanol on a glass surface at low pressures. The microlayer reflections were able to be viewed through the glass surface as to not constrain the bubble growth. The results indicated a wedge like microlayer profile with a thickness of under 1.0µm at a bubble radius of a few millimeters.

An early comprehensive study of the microlayer phenomenon was conducted by Cooper et al. (1969), who applied high speed photography along with an array of four rapid responding film thermocouples during nucleate boiling of toluene and isopropyl alcohol at low pressures. Direct surface temperatures were recorded as the base of the bubble advanced and then receded across the thermocouples. Figure 4 illustrates their results: the observed shape of the bubble (top graph), the observed temperature (middle graph), and the heat flux (bottom graph) with respect to time. From the temperature-time plot, a sharp drop in temperature occurred due to the evaporation of the microlayer, and then a temperature recovery followed as the dry spot formed. A relatively small drop in temperature indicated rewetting of the surface during the bubble’s departure. The heat flux was then determined by the integration of the conduction equation over the temperature-time plot showing a large amount of heat transfer during the microlayer evaporation and a relatively smaller amount of heat transfer as the bubble departs. An approximate boundary layer analysis was applied in order to estimate the microlayer thickness at any point in time during the bubble growth cycle:
\[ \delta(r) = C_c \sqrt{\nu_l t_g} \]  \hspace{1cm} (1)

where \( \nu_l \) is the liquid kinematic viscosity and \( t_g \) is the growth time required for the bubble to arrive at radius \( r \). The constant, \( C_c \), was determined experimentally to be 0.8.

Figure 4 – Results from Cooper et al. (1969)
Their calculated evaporation rate of the microlayer turned out to be on the same order of magnitude as the bubble growth rate concluding that the bubble gained a majority of its energy via microlayer evaporation.

A study to develop a measurement technique to obtain microlayer thickness for small, short lived bubbles pertaining to highly subcooled nucleate boiling was investigated by Koffman et al. (1983). By adopting the experimental method used by Jawurek et al. (1969), the time histories of the microlayer measured for ethanol and water indicated an almost wedge like shape. The initial microlayer thickness for water was measured at 1.85µm at a bubble radius of 0.25mm; the initial microlayer thickness for ethanol was about 1.6 times that of water. Similar to past observations, the microlayer thickness decreased as the bubble grew increasing the radius of the dry spot that forms underneath the bubble. The bubble growth rate of water was similar to the growth rate of an experiment that investigated the heat transfer associated with bubble formation in subcooled water, which was done by done Gunther et al. (1950). By comparing heat transfer data, Koffman et al. (1983) concluded that the evaporation of the microlayer alone cannot contribute to any more than half of the total heat transfer rate and that micro-convection must contribute an equal amount in nucleate boiling.

A more recent laser interferometry study with a high speed camera was completed by Gao et al. (2012), who investigated the microlayer beneath an ethanol vapor bubble during the bubble growth process. This experimental method studied the dynamic characteristics of the microlayer that included the movement of the gas-liquid-solid triple contact line, the micro-contact angle, bubble base radius, and the volume of the microlayer during nucleate boiling. In the beginning of the bubble growth cycle, the microlayer diameter increased rapidly increasing the microlayer volume from a time of 0.035ms to 0.599ms. Around 0.845ms, a dry spot
appeared, and the volume of the microlayer decreased due to its evaporation. Multiple correlations from the experimental data were obtained. A power law correlation for the triple contact line was obtained that included the dry spot radius and bubble growth time. The bubble base radius was correlated on a logarithmic scale showing that the bubble base radius increased rapidly before the dry spot appeared and much slower after the appearance of the dry spot. The growth of the microlayer was investigated during the initial bubble growth and after the dry spot appeared. The correlation from Cooper et al. (1969) was used for the initial bubble growth while a linear correlation was used after the dry spot appeared. Another linear relationship was obtained for the change in the micro-contact angle where it decreased as the bubble grows.

Measurements of the microlayer structure in nucleate boiling of water and ethanol at saturation conditions were completed by Utaka et al. (2013). A laser extinction method with a laser emission apparatus along with high speed camera was employed instead of laser interferometry. An optical fiber with a 94µm core diameter was located inside a thin metal tube that was placed in the liquid. Gas was flowed through the thin metal tube that surrounded the optical fiber so the growing bubble and gas would combine keeping the optical fiber from getting wet during the experiment. Even though this set up obstructs the bubble growth process, the microlayer thickness can be directly measured without contacting the superheated wall or investigation of fringe patterns from the laser interferometry approach. The laser measured the microlayer structure at a single radial location as the bubble advanced to its maximum bubble base. Then, the laser apparatus was moved to a new radial location and the experiment was conducted again to measure the microlayer structure. Each radial optical location displayed a wedge like microlayer structure as the bubble base advanced to its maximum radius. Due to the nature of the microlayer appearing and then evaporating quickly, the laser could potentially not
capture the equilibrium microlayer thickness as the bubble advances. An analytical method was developed for determining the equilibrium microlayer thickness based on the experimental results. The predicted equilibrium microlayer thickness was determined to increase linearly with an increase in radial distance from the bubble nucleation site, $r_L$, and agreed well with those measured in other studies. The relationship was developed as the following equations:

\[
\delta_0 = 4.46e^{-3} \times r_L \quad \text{for water} \\
\delta_0 = 10.2e^{-3} \times r_L \quad \text{for ethanol}
\]

The radial location of the equilibrium microlayer thickness for water and ethanol showed to be similar, but the thickness of ethanol was twice that of water. This study only investigated the microlayer structure as the bubble advanced to its maximum radial distance.

2.2 Numerical Models and Simulations

The mechanisms that contribute to bubble growth and the high heat transfer rates associated with nucleate boiling are complex. Numerical models and simulations can provide an insight into characteristics that are difficult to quantify analytically or through experiments. Lee et al. (1989) numerically simulated bubble growth and departure in saturated boiling of water that included the microlayer. The bubble was modeled to remain a truncated spherical shape throughout the growth cycle, and the microlayer thickness was represented by the formulation obtained by Cooper et al. (1969) in Eq. (1). The results indicated that the microlayer evaporation accounted for 87% of the total heat transfer during nucleate boiling. Due to the assumed truncated spherical profile, the bubble growth process that includes the bubble elongation, receding on the base wall, and necking prior to departure could not be captured.
Guo et al. (1994) developed a transient model to study evaporation of the liquid microlayer during nucleate boiling on the surface of a flat composite wall composed of a heated metallic foil and Pyrex glass substitute. The model was developed to simulate the evaporation of the microlayer that Koffman et al. (1983) observed in their bubble growth experiments. The model predictions agreed well with the trends that were observed experimentally for water. The results also indicated that the temperature of the heated surface was highly non-uniform. A parametric study was completed to investigate the effects of the wall thickness and thermal conductivity on the evaporation rate of the microlayer. It was found that the evaporation rate of the microlayer increased as either the wall thickness or thermal conductivity increased due to improved lateral heat conduction, approaching an isothermal wall [Guo et al. (1994)].

A model to calculate the heat transfer coefficients in nucleate boiling was presented by Stephan et al. (1994). The heat transfer and fluid flow surrounding a single bubble of R-114 on a copper plate was investigated by accounting for the meniscus curvature, adhesion forces, and thermal resistance at the interface. The results indicated a strong influence on the overall heat flow was due to the evaporation in the micro region and that molecular kinetic thermal resistance at the interface could not be neglected. The base length of the micro region for a single bubble of a radius of 0.125mm and a wall superheat of 3.5K came to be less than 1μm, but contributed to about 38% of the total heat transfer with a peak heat flux of 1550W/cm². When the wall superheat was increased to 4.2K, 60% of the total heat transfer passed through the micro region showing that wall superheat was a strong influence of heat transfer through the micro region. Although the full bubble growth process was not investigated, their prediction of heat transfer coefficients at a bubble radius of 0.125mm compared well with the experimental data provided in literature.
Dhir and his colleagues numerically simulated nucleate boiling including a microlayer model in a series of papers. A complete numerical simulation of a growing and departing bubble on a horizontal surface was modeled by Son et al. (1999). The computational domain was divided into two sections as the micro region and the micro region. The micro region consisted of the microlayer while the macro region contained the vapor bubble and neighboring liquid. A modified Level-Set method was employed to track the interface, which will be explained in Section 3.1. The microlayer equations included an augmented Young-Laplace equation to capture the pressure drop across the interface and a modified Clausius-Clapeyron equation to model the evaporation occurring at the interface, which were solved by applying the lubrication theory. The macro region solved the continuity equations to obtain the interface shape and position along with the temperature and velocity profiles. The solutions of the two regions were matched at a fixed location of the outer edge of the microlayer. The thickness of the microlayer was assumed to be 6e-10m with a fixed contact angle of 38°. The contribution of the microlayer was determined to be around 20% of the total heat flux throughout the simulation. The bubble growth prediction from the numerical simulation compared well with their experimental.

By extending the work of Son et al. (1999), Abarajith et al. (2002) numerically studied the effect of contact angle on the dynamics of a single bubble during pool boiling. Complete numerical simulations of a growing and departing bubble were carried out for a variety of contact angles and wall superheats. For every simulation, the contact angle was held constant as the bubble grew and departed on the horizontal wall. The results indicated the departing bubble diameter increased with a slight non-linearity as the contact angle increased for a given wall superheat. The non-linearity appeared to be greater with the increase in the wall superheat. The increase in contact angle increases the base area of the bubble in contact with the superheated
wall, which in turn enlarges the downward force from the surface tension. The vapor bubble must grow larger increasing its volume to overcome the additional force due to surface tension and eventually depart. For a given contact angle, an increase in wall superheat resulted in a greater departure diameter and a faster departure time. The microlayer heat transfer rates increased substantially when the contact angle increased due to the additional base area. The same trend was also seen in the macro region heat transfer, due to large bubble diameters and growth periods associated with larger contact angles.

A dynamic microlayer model to predict heat flux including the critical heat flux in fully developed nucleate boiling of water at atmospheric pressure was proposed by Zhao et al. (2002). The heat transfer associated with boiling was mainly due to the evaporation of the microlayer neglecting the macro region heat transfer from the superheated wall. The microlayer thickness, dryout area, and heat flux were all determined as functions of wall superheat in order to create a predicted boiling curve. The equilibrium thickness of the microlayer was found to become thinner when the wall superheat was increased consequently increasing the local evaporation and dryout speed. They predicted a maximum heat flux on their boiling curve of $1.2 \times 10^6 \text{W/m}^2$ at a wall superheat of about 20.9K. The predicted CHF results matched relatively well with experimental data found in literature.

The lateral merger of vapor bubbles during nucleate boiling was numerically simulated by Mukherjee et al. (2004). As a colleague of Dhir, the Level-Set method was implemented for interface tracking along with the microlayer methodology from previous studies. The numerical study involved the merger of two and three bubbles at various orientations that include in a line and a plane. The numerical results indicated that a vapor bridge formed at the early merger process of the bubbles trapping liquid under the bridge and vapor tails during the later stage of
the merger. Due to the trapping of the liquid under the bridge, the heat transfer from wall increased as the cooler liquid was drawn close to the superheated wall during the contractions as the bubbles merge together. The highest heat transfer was obtained from the merger of three bubbles in a plane. The wall heat transfer associated with the merger of multiple bubbles was determined to be significantly higher than a single bubble. The bubble shape and growth rate predicted from the numerical simulations showed good agreement with their experimental data.

Liao et al. (2004) developed a model to investigate the influence of heat transfer through the bulk liquid thermal boundary layer and the microlayer on bubble growth in saturated nucleate boiling. The heated surface was kept at a constant temperature and the microlayer was assumed to have a linear profile. The numerical solutions for the temperature of the liquid surrounding the hemispherical bubble indicated the presence of a thin thermal boundary layer adjacent to the dome of the bubble. Heat transfer from the microlayer underneath the bubble and the superheated bulk liquid through the bubble cap promoted rapid bubble growth early in the bubble’s growth cycle. The thermal boundary layer contributed a significant amount of heat transfer from the bulk liquid into the vapor bubble and could potentially be greater than the heat transfer from the microlayer. The heat transfer through the bubble cap was found to depend on the thickness of the superheated liquid. The model resulted in 70% of the heat transferred to the bubble was through the dome via the superheated liquid layer within a timeframe of 0.8ms. The solution was consistent with the experimental data obtained by Yaddanapudi et al. (2001).

Fuchs et al. (2006) introduced a transient model to numerically simulate the growing, detaching, and rising of a single propane/n-butane bubble during nucleate boiling. The model required that a waiting period between two successive bubbles to be entered as an input parameter. A spherical bubble shape was assumed throughout the entire growth period of the
bubble cycle from the initial hemispherical bubble to departure neglecting the bubble elongation and necking process while a free surface was assumed after departure as the bubble ascended in the bulk liquid. The heat transfer associated with the micro region was determined using a one dimensional heat transfer model. The macro region used a two dimensional heat conduction and convection model to determine the heat transfer from the superheated bulk liquid. Approximately 63% of the total heat transfer occurred during the bubble growth and detachment process, while the remaining 37% occurred during the bubble rise due the superheated wall conducting heat into the bulk liquid. The transient model predicted that 32% of heat flowed through the micro region during the bubble growth and departure process. The predicted heat transfer coefficients were 12% less when compared to experimental results.

The dynamic contact angle of single bubbles during nucleate boiling was investigated numerically by Mukherjee et al. (2007). The Level-Set method was implanted to track the interface. For numerical simplification, the evaporation from the microlayer was excluded to focus on the liquid motion and surface wettability characteristics. Modeling the contact angle using the contact line velocity caused the triple point to stick and slip compared to a continuous motion when a static contact angle was applied causing an over prediction of the departure time. The advancement of the contact angle contributed more the bubble growth rate as opposed to when the contact angle receded. In the absence of experimental data, a static contact angle can be applied, but good engineering judgment must be used when choosing that value. Applying an average value of the advancing/receding contact angle can under predict the bubble departure volume; however, numerical modeling using measurements from experiments proved that there was a slight influence on the vapor volume growth rate when employing a static contact angle compared to a dynamic contact angle [Mukherjee et al. (2007)].
Heat transfer in the microlayer under a bubble during nucleate boiling was investigated numerically by Christopher et al. (2010). The model developed by Son et al. (1999) was further advanced by using a similar set of equations, but applied more realistic boundary conditions. The theoretical model predicted the microlayer profile and heat transfer rates for water and FC 72. The effects of the wall superheat, Hamaker constant, bubble size, and accommodation coefficient on the microlayer characteristics were investigated. The microlayer profiles and heat flux variations were calculated for different wall superheats at the same bubble radius with the results indicating that the microlayer radial distance and maximum thickness becomes smaller with the increase in wall superheat. The predicted heat fluxes showed a sharp spike close to the inner boundary of the microlayer and then decreasing with radial distance. At higher wall superheats, a steeper slope was seen as the heat flux reached its significantly higher peak during the spike. The total heat transfer increased as the bubble grew in size; however, there was little change in the maximum heat flux at the peak of the spike. The Hamaker constant was shown to have a minimum effect on the heat flux. The ideal accommodation coefficient produced an 8% increase in total heat transfer compared to a more acceptable water accommodation coefficient of 0.03; however, the predicted heat fluxes for a wall superheat of 1K and 10K with an ideal accommodation coefficient compared well with the heat fluxes that were determined by solving the complete Navier-Stokes equations in the microlayer.
3.1 Numerical Approach

To computationally simulate nucleate bubble growth from incipience to departure on a heated surface, the domain is divided into two regions: the micro region and the macro region, as shown in Figure 3 and Figure 5. The micro region contains the thin liquid layer that forms underneath the vapor bubble, adjacent to the heated surface whereas the macro region contains the vapor bubble and the neighboring bulk liquid. The length scale of the micro region covers the range of nanometers to micrometers, and the macro region has length scales from micrometers to millimeters. Looking at Figure 3 and Figure 5, the location of the microlayer in the macro region appears to coincide with the intersection of the liquid vapor interface and the heated surface.

Figure 5 – Macro and Micro Regions
The system of equations that govern the dynamics of the thin liquid layer in the micro region developed by Christopher et al. (2010) is implemented to determine the heat transfer and phase change occurring near the contact line. This method investigates the microlayer characteristics for a variety of superheats at multiple bubble radii. The mass transfer contribution to bubble growth from the microlayer during nucleate boiling is represented as a source term in the governing equations of the macro region.

The numerical solution of bubble formation in the macro region involves solving the incompressible Navier-Stokes equations and energy equation over the liquid and vapor domains to capture the moving interface. Characteristics of nucleate boiling depend heavily on accurately tracking of the dynamic liquid vapor interface. Two approaches for interface tracking have been applied over the years, one being the Volume-of-Fluid (VOF) and other being the Level-Set methods. The Level-Set method defines the interface by a signed distance function in which a positive sign represents one phase while a negative sign represents the other phase and the zero level set identifying the interface [Osher et al. (1988)]. Sussman et al. (1994) applied the Level-Set approach for tracking the interface of two adiabatic incompressible fluids. Dhir and his colleagues have implemented the Level-Set method for numerous boiling simulations that include vapor stems, single bubble, lateral merger of bubbles, and an evaporating meniscus on a moving heated surface. A major drawback to this interface tracking method is the numerical diffusion resulting in poor conservation of mass requiring an additional interface-preserving algorithm to help overcome this obstacle.

This computational study employs the VOF method developed by Hirt et al. (1981) to capture the dynamic interface of two immiscible fluids by applying a scalar function throughout the domain where the scalar is known as the volume fraction. The volume fraction denotes the
volume ratio of the phases present within each control volume where the volume fraction of each phase sums to unity. Variables and properties are shared by the phases as volume-averaged values. Unlike the Level-Set method, the VOF model conserves mass precisely. The VOF model consists of an interface reconstruction scheme to define the interface in each multi-phase cell based on the volume fraction, an advection algorithm to calculate the volume fraction at the next time step using the reconstructed interface and velocity field, and a surface tension model to account for the effects of surface tension at the interface. The treatment of surface tension is based on the continuum surface tension model by Brackbill et al. (1992), which converts the surface tension force into a volumetric source term represented in the momentum equation.

The macro governing equations along with the volume fraction equation include source terms that occur at the interface and are solved throughout the domain. In the continuity equation, the mass source terms represents the mass transfer during evaporation. The energy equation also has source terms to balance the heat transfer from the phase transition due to mass transfer. This computational study employs two mass transfer modes that consist of the microlayer modeled by Christopher et al. (2010) and a phase change model that occurs due to the heat transfer from the superheated liquid layer near the heated surface, also called transient conduction model. Each method has their own set of source terms represented in the macro region governing equations. The following sections discuss the detailed numerical approach for the micro region and macro region along with the computational set up, boundary conditions, and solution parameters employed to simulate nucleate boiling from inception to departure.
3.2 Micro Region

3.2.1 Microlayer Mathematical Formulation

As stated before and shown in Figure 3 and Figure 5, the micro region consists of the thin liquid film that lies between the vapor bubble and the heated surface. In order to obtain the contribution to bubble growth from the microlayer during nucleate boiling, the heat transfer and microlayer profiles are determined using the method derived by Christopher et al. (2010). This model solves the conservation equations within the liquid microlayer assuming steady-state and laminar conditions. Son et al. (1999) validated the assumption of constant fluid properties in each phase such as density, viscosity, and thermal conductivity for low superheats. The microlayer is thin relative to its length allowing for the assumption that evaporation occurs only in the direction normal to the interface. This simplification may be less accurate for the outer thicker part of the microlayer; however, the heat transfer in this region is much less than the thin inner section. This provides a heat flux and liquid velocity relation at the interface given by:

$$q'' = \rho_l h_f v(\delta)$$  \hspace{1cm} (3)

where $v(\delta)$ is the liquid velocity normal to the interface and $\delta$ is the microlayer thickness.

Solving the governing equations within the microlayer starts with expressing the mass conservation equation in radial coordinates:

$$\frac{1}{r} \frac{\partial}{\partial r} (ru) + \frac{\partial v}{\partial y} = 0$$  \hspace{1cm} (4)

Due to the layer being thin relative to its length, lubrication theory is used to describe the fluid flow within the microlayer defined as:
Integrating the momentum equation, Eq. (5), from the heated surface \((y = 0)\) to the interface \((y = \delta)\) with the boundary conditions that the velocity at the heated surface is zero and the shear stress at the interface is zero describes the fluid flow in the radial direction as:

\[
\frac{\partial P_l}{\partial r} = \mu_l \frac{\partial^2 u}{\partial^2 r} \tag{5}
\]

Substituting Eq. (6) into the continuity equation, Eq. (4), and integrating again from the heated surface to the interface gives an expression for the liquid velocity normal to the interface:

\[
u(\delta) = \frac{\delta^3}{3r\mu_l} \frac{\partial}{\partial r} \left( r \frac{\partial P_l}{\partial r} \right) \tag{7}
\]

The heat transfer through the liquid microlayer in the vertical direction can be described by Fourier’s Law stating the heat flux as:

\[
q'' = k_l \frac{(T_w - T_{int})}{\delta} \tag{8}
\]

The evaporative heat flux of the liquid microlayer can be expressed by using a modified Clausius-Clapeyron equation, which includes the temperature change and pressure drop across the liquid vapor interface:

\[
q'' = h_{ev} \left[ T_{int} - T_v + \frac{(P_l - P_v)T_v}{\rho_v h_{fg}} \right] \tag{9}
\]

where \( h_{ev} \) is the evaporative heat transfer coefficient that can be explained using the kinetic theory of gases:
The evaporation and condensation accommodation coefficient, $\beta$, accounts for the behavior of the vapor molecules in their reflective collisions with the liquid surface. The temperature of the vapor equates to the saturation temperature at the vapor pressure:

$$T_v = T_{\text{sat}}(P_v)$$

(11)

The pressure of the liquid and vapor phases are described by a modified augmented Young-LaPlace equation:

$$P_l = P_v - \sigma \kappa - \frac{A}{\delta^3} + \frac{q''r^2}{\rho_v h_f^2}$$

(12)

The second term on the right side of Eq. (12) represents the capillary pressure caused by the curvature, $\kappa$, where $\sigma$ is the surface tension. The third term is for the disjointing pressure containing the Hamaker constant, $A$, which accounts for van der Walls forces between the wall and liquid. The final term originates from the recoil pressure due to the departing vapor molecules at the interface. According to the results provided by Christopher et al. (2010), the recoil pressure term has a negligible effect on the heat flux and the total heat transfer from the microlayer; therefore, it will be neglected in this study. The curvature of the liquid vapor interface is defined as:

$$h_{ev} = \frac{2\beta h_f^2 \rho_v}{2 - \beta} \frac{\bar{M}}{T_v} \left( \frac{\bar{M}}{2\pi R T_v} \right)^{\frac{1}{2}} \left[ 1 - \frac{P_v}{2h_f \rho_v} \right]$$

(10)
The temperature of the liquid vapor interface is determined by the combination of Fourier’s Law in Eq. (8) and the evaporative heat flux in Eq. (9) along with the pressure balance of Eq. (12) resulting in the following equation with the constant $C$:

$$T_{int} = \frac{k_l T_w + h_{ev} T_v + C \sigma \kappa + C \frac{A}{\delta^3}}{k_l \delta + h_{ev}}$$  \hspace{1cm} (14)

$$C = \frac{h_{ev} T_v}{\rho_v h_{fg}}$$

The combination of Eq. (3) and Eq. (7) gives an expression for heat flux at the interface as a function of the liquid pressure gradient where the pressure balance, Eq. (12), can be differentiated to derive an expression related to curvature:

$$\kappa'' = \frac{1}{\sigma} \ast G(\delta)$$  \hspace{1cm} (15)

where the prime denotes differentiation with respect to $r$ and the function $G(\delta)$ can be defined as:

$$G(\delta) = -\frac{3\mu_l q''}{\rho_l h_{fg} \delta^3} - \frac{\sigma \kappa'}{r} + 3 \frac{A}{r \delta^5} \delta' + 3 \frac{A}{\delta^4} \delta'' - 12 \frac{A}{\delta^5} \delta'^2$$  \hspace{1cm} (16)

The second derivative with respect to $r$ of the interfacial curvature, Eq. (13), gives the following equation:
\[ \kappa'' = \frac{\delta'''}{(1 + \delta'^2)^2} + F(\delta) \]  

(17)

where the function \( F(\delta) \) can be defined as:

\[
F(\delta) = \frac{2\delta'}{r^3(1 + \delta'^2)^{\frac{1}{2}}} + \frac{r\delta''' - 2\delta''}{r^2(1 + \delta'^2)^{\frac{3}{2}}}
- \frac{3\delta'\delta''^2 + 3r\delta''' + 9r\delta'\delta''\delta'''}{r(1 + \delta'^2)^{\frac{5}{2}}} + \frac{15\delta'^2\delta'''^3}{(1 + \delta'^2)^{\frac{7}{2}}}
\]  

(18)

Combining Eq. (15) and Eq. (17) results in a fourth-order ordinary differential equation for the liquid microlayer thickness:

\[
\delta'''' = \left[ \frac{G(\delta)}{\sigma} - F(\delta) \right] (1 + \delta'^2)^{\frac{3}{2}}
\]  

(19)

The equilibrium microlayer thickness, \( \delta_0 \), during nucleate boiling originates when the van der Walls forces between the heated surface and superheated liquid become strong enough to prevent evaporation. The non-evaporating region is flat with no curvature and the interface temperature matches that of the wall inhibiting heat transfer. Setting the evaporative heat flux in Eq. (9) to zero and applying the pressure balance equation, Eq. (12), with the curvature being zero, gives the equilibrium microlayer thickness to be:

\[
\delta_0^3 = \frac{AT_v}{(T_w - T_v)\rho_v h_{fg}}
\]  

(20)

Determining the microlayer profile from Eq. (19) and other microlayer characteristics requires a detailed methodology with a set of boundary conditions.
3.2.2 Microlayer Methodology

Solving the fourth-order governing equation of Eq. (19) is quite difficult due to the rapid change in the magnitude of the terms especially as the microlayer thickness becomes very small. The fourth-order governing equation is solved by employing a fourth-order Runge-Kutta scheme in the radial direction with appropriate boundary conditions.

![Microlayer Diagram](image)

Figure 6 – Micro Region

Looking at micro region in Figure 6, the boundary conditions for Eq. (19) are as follows:

\[
\begin{align*}
\delta(R_0) &= \delta_0, \quad \delta'(R_0) = 0, \quad \delta''(R_0) = 0, \\
\delta'(R_{\text{max}}) &= \tan \theta, \quad \delta'''(R_{\text{max}}) = 0
\end{align*}
\]  

(21)

where \( R_{\text{max}} \) is defined with the bubble radius, \( R_b \), as:

\[
R_{\text{max}} = R_b \sin \theta
\]  

(22)

The fourth-order differential equation of Eq. (19) requires just four boundary conditions to be solved; however, a fifth boundary condition is needed to define the location of \( R_0 \), which is where the equilibrium microlayer thickness, \( \delta_0 \), is reached.
According to the methodology provided by Christopher at al. (2010), the integration of Eq. (19) using the fourth-order Runge-Kutta scheme starts at $R_{\text{max}}$ and moves inward towards $R_0$, which is unknown initially. This approach requires the addition of two more boundary conditions for $\delta$ and $\delta''$ at $R_{\text{max}}$ in conjunction with the two listed in Eq. (21). $\delta(R_{\text{max}})$ was chosen such that $\delta'(R_0)$ went to zero and $\delta''(R_{\text{max}})$ was chosen such that $\delta''(R_0)$ went to zero to satisfy all the boundary conditions in Eq. (21) [Christopher et al. (2010)]. The location of $R_0$ is defined where $\delta$ reaches $\delta_0$ ending the Runge-Kutta integration: $\delta(R_0) = \delta_0$.

The governing equation for the microlayer thickness in Eq. (19) is similar to that of Dhir and his colleagues, but neglecting the recoil pressure term; however, the boundary conditions in Eq. (21) differ. Dhir and his colleagues selected $R_0$ and $\delta''(R_0)$ so that the outer edge of the microlayer was also fixed, and became nearly normal to the surface by selecting values of $\delta''(R_0)$ for a reasonable prediction of the liquid-vapor interface. The final difference in boundary conditions was regulating $\delta''(R_0)$ to be zero. This would affect the heat transfer due to the curvature effects when the microlayer thickness became very thin reaching the equilibrium microlayer thickness of $\delta_0$ [Christopher et al. (2010)].

Once the integration using the Runge-Kutta scheme is complete, the heat transfer rate at the wall from the micro region can be determined by the following expression:

$$Q_{\text{ml}} = \int_{R_0}^{R_{\text{max}}} 2\pi r \frac{k_l(T_w - T_{\text{int}})}{\delta} dr$$

(23)

The integration method for Eq. (23) was done by summing the local heat transfer rate at each radial step in the Runge-Kutta scheme from $R_0$ to $R_{\text{max}}$. The total heat transfer rate from Eq. (23) is the quantity necessary for expressing the mass source term in the macro region. The
methodology used here determines the total heat transfer rate, $Q_{mt}$, for a microlayer profile at a specific bubble radius. Due to transient nature of nucleate boiling, the microlayer profile changes as the bubble diameter increases. To compensate for this, Eq. (19) was solved multiple bubble radii for a given wall superheat to create an expression to relate the total heat transfer rate and bubble radius:

$$Q_{mt} = f(R_b)$$  \hspace{1cm} (24)

Dividing Eq. (24) by the latent heat of vaporization gives the mass flow rate of the liquid evaporating into vapor at the interface for a particular bubble radius that is determined by function for the total heat transfer rate:

$$m'(R_b) = \frac{Q_{ml}(R_b)}{h_{fg}}$$  \hspace{1cm} (25)

This expression is to be calculated at every time step throughout the simulation saving computational time as opposed to running fourth-order Runge-Kutta scheme at each time step. The following section will explain the VOF method for interface tracking, the macro region governing equations that include the volumetric source terms, and the derivation of these volumetric source terms.
3.3 Macro Region

3.3.1 Volume-of-Fluid (VOF) Method

The VOF model tracks the interface between different phases by calculating the volume fraction in each control volume or cell throughout the domain. For the $p$th phase, the volume fraction in a cell, $\alpha_p$, has three possible conditions:

$\alpha_p = 0$: the cell is empty of the $p$th phase

$\alpha_p = 1$: the cell is full of the $p$th phase

$0 < \alpha_p < 1$: the cell contains the interface between the $p$th phase and one or more phases

In each cell, the volume fraction of each phase must sum to unity. In the current study, there are two phases: vapor and liquid. When $\alpha_v = 1$ or $\alpha_l = 0$, it represents the vapor region, also known as the primary phase; when $\alpha_l = 1$ or $\alpha_v = 0$, it represents the liquid region, also known as the secondary phase. The interface of the two phases is represented when $0 < \alpha_v < 1$ or $0 < \alpha_l < 1$. In the transport equations, properties and variables are assigned as volume average values based on the local value of $\alpha_p$ in each cell throughout the domain. If the volume fraction of liquid, the secondary phase, was being calculated and tracked throughout the domain, density and viscosity are determined in each cell as follows:

$$\rho = \alpha_l \rho_l + (1 - \alpha_l) \rho_v$$

$$\mu = \alpha_l \mu_l + (1 - \alpha_l) \mu_v$$

(26)

All properties are calculated in a similar fashion and are constant within their respective phase. Properties for individual phases are based on their respective volume fraction.
In the VOF model, the dynamic interface is captured by the solution of the volume fraction continuity equation in each cell throughout the domain. For the $p$th phase, this equation takes the following form:

$$\frac{\partial \alpha_p}{\partial t} + \nabla \cdot (\alpha_p \mathbf{u}_p) = \frac{S_{m_p}}{\rho_p}$$

(27)

where $S_{m_p}$ represents the volumetric mass source terms that will simulate the evaporative mass transfer. For the cells located at the interface, a geometric reconstruction (Geo-Reconstruction) scheme is used to obtain accurate face flux values. Rider et al. (1998) applied a generalized geometric reconstruction scheme for structured and unstructured meshes where the interface between fluids is denoted by a piecewise-linear interface calculation (PLIC). A linear slope represents the interface between two fluids within each cell and applies its lined shape to determine the advection of the fluid over the faces of the cell. The geometric reconstruction scheme consists of three steps. The first step computes the location of the linear interface comparative to the center of each partially filled cell depending on its volume fraction and derivative. The second step determines the quantity of fluid advecting through each face using the linear interface and tangential/normal velocity distribution on the face. The final step determines the volume fraction in the cell by applying a flux balance that was founded during the prior step.

### 3.3.2 Governing Equations

Along with the volume fraction equation, the incompressible Navier-Stokes equations and energy equation are solved throughout the domain. The continuity equation is similar to the volume fraction equation and can be expressed as:
\[ \nabla \cdot (\overline{u_p}) = \frac{S_{mp}}{\rho_p} \]  

(28)

The momentum equation shares the velocity field among the phases and calculates the properties according to Eq. (26) taking the following form:

\[ \frac{\partial (\rho \overline{u})}{\partial t} + \nabla \cdot (\rho \overline{u} \overline{u}) = -\nabla P + \nabla \cdot [\mu(\nabla \overline{u} + (\nabla \overline{u})^T)] + \rho \overline{g} + \overline{F}_{\sigma} \]  

(29)

where \( \overline{F}_{\sigma} \) is the volumetric source term for surface tension force at the liquid vapor interface. The surface tension approach used in this study is the continuum surface force (CSF) model proposed by Brackbill et al. (1992). As per this model, the pressure drop across the surface depends on the surface tension coefficient and the surface curvature measured by two radii in orthogonal directions, \( R_1 \) and \( R_2 \), as:

\[ P_2 - P_1 = \sigma \left( \frac{1}{R_1} + \frac{1}{R_2} \right) \]  

(30)

where \( P_1 \) and \( P_2 \) denote the pressures in the two phases. The surface curvature is computed from local gradients in the surface normal at the interface. The surface normal is defined as:

\[ n = \nabla \alpha_p \]  

(31)

The surface curvature, \( \kappa \), is defined in terms of the divergence of the unit normal, \( \hat{n} \), as:

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

(32)

where the unit normal is defined as:
The surface tension force is converted into a volumetric force by using a divergence theorem. If two phases are present in a cell, the volumetric source term for the surface tension force that appears in the momentum equation of Eq. (29) is given by:

$$\vec{F}_o = \sigma \frac{\rho \kappa \nabla \alpha_p}{2 (\rho_l + \rho_v)}$$  \hfill (34)

The governing equation set is completed by the energy conservation equation that is also shared among the phases given by:

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\overline{u} (\rho E + P)) = \nabla \cdot (k_{ef} \nabla T) + S_{Ep}$$  \hfill (35)

where $S_{Ep}$ is the energy source term required to simulate the heat transfer between phases during evaporation. The properties $k_{ef}$ and $\rho$ are shared among the phases similar to the momentum equation. Energy, $E$, and temperature, $T$, are treated as mass-averaged values taking the following form:

$$E = \frac{\sum_{p=1}^{n} \alpha_p \rho_p E_p}{\sum_{p=1}^{n} \alpha_p \rho_p}$$  \hfill (36)

The energy for each phase is based on the specific heat of that phase and the shared temperature. The required volumetric source terms are determined based on the two mass transfer modes used in this computational study.
3.3.3 Source Terms

In order to simulate nucleate boiling, volumetric source terms are included in the macro governing equations. The mass source terms in the continuity equation represent the mass transformation from liquid to vapor, while the energy source terms in the energy equation balance the heat transfer that the mass source terms produce during their transformation. The continuity equation will have volumetric mass source terms for both the liquid and vapor phases. The energy equation is shared among the phases as must its volumetric energy source terms. As stated earlier, a microlayer model and phase change model are employed as the contributing factors to bubble growth. The microlayer model calculates its contribution to the source terms on a per cell basis that is incorporated into the phase change model. This method derives a set of source terms that are incorporated in the conservation equations and solved in the macro region.

A phase change is employed due to the heat transfer from the superheated liquid surrounding the bubble base near the wall contributing to bubble growth during nucleate boiling. This model uses a simple conduction heat transfer equation to obtain the volumetric source terms for the continuity and energy equations:

\[ q'' = k_i \nabla T \]  (37)

In order to apply the phase change model, the source terms in the continuity equation must be volumetric in the correct units of kg/m³s. By dividing the heat flux by the latent heat of vaporization, an expression for the mass flux occurring at the interface where the liquid evaporates into vapor:
The mass flux for the phase change source term in Eq. (38) is converted into an equivalent volumetric mass transfer source term by applying a similar technique that Brackbill et al. (1992) used in his CSF model.

![Figure 7 – The Interface Region [Deodhar et al. (2012)]](image)

Figure 7 displays the volume fraction of liquid where the interface is represented as the region that has a volume fraction value in-between 0 and 1. Typically, the interface region varies from consisting of 1 to about 4 computational cells within the mesh during the simulation. This creates a non-ideal “zero thickness” interface surface. The discontinuity of the two phases is replaced by a continuous model that changes a property gradually between the phases using the Gauss-divergence theorem. In this study, the volume fraction scalar is used to smooth the transition of the mass transfer over the interface. Using the CSF method, the mass flux

\[
m_{tc}'' = \frac{q''}{h_{fg}} = \frac{k_i \nabla T}{h_{fg}}
\]
conversion derives the phase change due to transient conduction as a volumetric mass source term in the volume fraction and continuity equations:

\[
S_{tc,m_p} = m'_{tc} \frac{\nabla \alpha_l \cdot \alpha_l}{[\alpha_l] \langle \alpha_l \rangle}
\]  

(39)

where \(\alpha_l\) is the volume fraction of liquid in that cell and:

\[
\begin{align*}
[\alpha_l] &= \alpha_{l,max} - \alpha_{l,min} = 1 - 0 = 1 \\
\langle \alpha_l \rangle &= \frac{(\alpha_{l,max} + \alpha_{l,min})}{2} = \frac{(1 + 0)}{2} = \frac{1}{2}
\end{align*}
\]

(40)

Cells that are on the interface consist of liquid and vapor based on their respective volume fraction value. During simulated boiling, vapor is added and liquid is subtracted in the interface cells. Since the calculation of phase change mass flux, \(m'_{tc}\), in Eq. (25) is always positive, the vapor phase change due to transient conduction takes the following form as the vapor mass source term:

\[
S_{tc,m_v} = 2\alpha_l \nabla \alpha_l \cdot m''_{tc} = 2 \alpha_l \nabla \alpha_l \frac{k_l \nabla T}{h_{fg}}
\]

(41)

The microlayer contribution to bubble growth during nucleate boiling originates from the mass flow rate of the evaporating liquid in Eq. (25), which includes the total heat transfer rate. Once again, the source terms in the continuity equation must be volumetric in the correct units of \(\frac{kg}{m^3 s}\). In order to get the mass flow rate into the correct units for the continuity equation, Eq. (25) is divided by the volume of liquid that it is being applied at and since this equation is always positive, it becomes the vapor microlayer mass source term taking the following form:
Due to the instabilities created by applying the microlayer source terms to the cells adjacent to the base wall, the numerical value of the vapor microlayer mass source term from Eq. (42) is added into the phase change transient conduction source term. For this method to be employed, the mass flow rate is divided by the volume where the phase change source term is to be applied. This is done by adding the cell volumes where the temperature gradient is not equal to zero. With this methodology, the total volumetric vapor mass source term can be expressed in the following form:

\[ S_{m_v} = S_{tcv} + S_{vim} \]

\[ S_{m_v} = 2\alpha_1\nabla\alpha_1 \frac{k_l\nabla T}{h_f} + \frac{Q_{ml}(R_b)}{h_f V_{liq}} \]  \hspace{1cm} (43)

The same amount of vapor added must be subtracted out from the liquid deriving the total liquid mass source term as:

\[ S_{m_l} = -S_{m_v} \]  \hspace{1cm} (44)

The energy source term is shared among the phases in the energy conservation equation and must be volumetric in the correct units of \( \frac{W}{m^3} \). This source term balances the heat transfer when liquid is transformed into vapor in terms of enthalpy defining the total energy source term as:

\[ S_E = -S_{m_v}[h_f + (\alpha_l C_{p,l} - \alpha_v C_{p,v})(T_{sat} - T_{ref})] \]

\[ (45) \]

where \( C_{p,l} \) and \( C_{p,v} \) are the specific heats at constant pressure of liquid and vapor, respectively. \( T_{ref} \) is the reference temperature held constant at 298.15K and used for the enthalpy calculations.
3.3.4 Computational Procedure

From multiple experimental studies of nucleate boiling, it has been observed that the bubble develops in a spherical and symmetrical shape. Therefore, 2D axisymmetric transient settings are used for the simulation.

As shown in Figure 8, the computational domain is zoomed in for clarification and consists of a small cavity and a hemispherical vapor bubble patched. The boundary conditions are as follows:

1. Walls have a no slip condition:
   \[ \ddot{u} = 0 \]

2. Pressure Outlet has a zero gauge condition:
   \[ P_{out} = 0 \]

3. Axis has a zero flux:
\[ \nabla \phi = 0 \]

The mesh size carried out for this computational study is an 8mm by 8mm domain that consists of two subdivisions. The primary section of the mesh where the bubble growth process occurs has a uniform structured section of 300µm x 600µm with an aspect ratio of 1. This was chosen to capture the full bubble growth process that starts with a small hemispherical bubble with a diameter at 60µm and ends with the necking of the fully developed bubble just prior to departure. The outer section of the mesh is unstructured and a necessary part of the domain so that the bubble growth cycle is not affected by the boundaries. A cell distance of 5µm was decided for the uniform structured subdivision due to the extremely small microlayer thickness, the small initial hemispherical bubble size, and to capture a smooth necking process.

The governing equations are solved using a second-order upwind implicit discretization scheme for space. The transient formulation was solved using a first-order implicit discretization. Pressure Implicit with Splitting of Operators (PISO) scheme was applied for the coupling of pressure and velocity. The Geo-Reconstruction scheme explained in Section 3.3.1 was applied for the interface reconstruction of the volume fraction scalar. The solution was obtained by keeping a Global Courant Number of 0.2 with a variable time stepping method. The time step is adjusted at the beginning of each iteration in order to keep the Global Courant Number low helping to improve the numerical stability of the solution.
RESULTS AND DISCUSSIONS

4.1 Overview

The results and discussions of this computational study are divided into two sections. The first section investigates the microlayer characteristics that include the microlayer profile, heat flux, and total heat transfer rate for various wall superheats and bubble radii. The second section displays the results of single bubble simulations in nucleate boiling that predict the bubble shape, temperature profiles, growth rate, and departure diameter. The single bubble simulation studies aim to investigate the bubble growth dynamics in pure saturated water and in aqueous surfactant solutions. Surfactants are introduced to provide an understanding of the role that dynamic surface tension and surface wettability play in bubble growth dynamics during nucleate pool boiling.

4.2 Microlayer

The governing equation for the microlayer thickness underneath the vapor bubble is represented by the fourth-order ordinary differential equation in Eq. (19). By applying the boundary conditions in Eq. (21), the microlayer boundary layer profile and heat transfer rates at the interface can be determined for a variety of superheats and bubble radii. In order to obtain the results for the microlayer characteristics, a large number of step sizes was applied in the fourth-order Runge-Kutta scheme due to the rapid change of the terms in Eq. (19) as the microlayer thickness reaches its equilibrium value. The results of the Runge-Kutta scheme were calculated by using constant properties of liquid and vapor at saturated conditions of water as shown in Table 1. Other properties including a contact angle of 38°, the Hamaker constant of
1x10^{-20}\text{N} \cdot \text{m}, and a evaporation and condensation accommodation coefficient of unity were chosen in order to compare the results determined by Christopher et al. (2010) with the microlayer characteristics calculated in this study.

Table 1 – Properties of Saturated Water at 373.15K

<table>
<thead>
<tr>
<th>Properties</th>
<th>Liquid</th>
<th>Vapor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Latent Heat: kJ/kg</td>
<td>2257</td>
<td></td>
</tr>
<tr>
<td>Surface Tension: N/m</td>
<td>0.0589</td>
<td></td>
</tr>
<tr>
<td>Density: kg/m$^3$</td>
<td>957.85</td>
<td>0.5956</td>
</tr>
<tr>
<td>Specific Heat (press): J/(kg·K)</td>
<td>4217</td>
<td>2029</td>
</tr>
<tr>
<td>Thermal Conductivity: W/(m·K)</td>
<td>0.68</td>
<td>0.0248</td>
</tr>
<tr>
<td>Dynamic Viscosity: kg/(m·s)</td>
<td>2.79x10^{-4}</td>
<td>1.202x10^{-3}</td>
</tr>
</tbody>
</table>

In order to solve the microlayer thickness profiles from Eq. (19), the equilibrium microlayer thickness, $\delta_0$, needs to be determined by Eq. (20). This provides a necessary boundary condition at the equilibrium microlayer radial distance of $R_0$ in Eq. (21); the results are shown based on the wall temperature in the following Table 2:

Table 2 – Equilibrium Microlayer Thickness

<table>
<thead>
<tr>
<th>Wall Superheat: K</th>
<th>$\delta_0$: m</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 (375.15K)</td>
<td>1.12x10^{-9}</td>
</tr>
<tr>
<td>4 (377.15K)</td>
<td>8.85x10^{-9}</td>
</tr>
<tr>
<td>6 (379.15K)</td>
<td>7.73x10^{-9}</td>
</tr>
<tr>
<td>8 (381.15K)</td>
<td>7.02x10^{-9}</td>
</tr>
</tbody>
</table>

The equilibrium microlayer thickness was determined on the order of nanometers and appears to decrease with an increase in wall superheat. By applying the appropriate boundary conditions, the microlayer thickness profiles were determined for water at various wall superheats for a bubble radius of 0.1mm and shown in Figure 9. The microlayer profile began at the maximum microlayer radial distance of $R_{\text{max}}$ and approached the equilibrium microlayer thickness at $R_0$. 

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The microlayer thickness at $R_{\text{max}}$ became smaller as the wall superheat increased. According to Christopher et al. (2012), the microlayer thickness at $R_{\text{max}}$ must be a function of the properties and the wall superheat to properly satisfy the boundary conditions in Eq. (21). Previous models assumed a value of the microlayer thickness at $R_{\text{max}}$ leading to results that are not compatible with the physics. The slope of the microlayer profile at $R_{\text{max}}$ started at the same value for all wall superheats; however, sharper curvature can be seen near $R_0$ for higher wall superheats. The curvature reached a maximum near $R_0$ when the microlayer approached its equilibrium thickness. The calculated microlayer profiles in this study compared well with results by Christopher et al. (2010), but were shifted a little to the left. This can be due to the rapid change in magnitude of the parameters as the integration for the microlayer thickness in Eq. (19) approached the boundary conditions at $R_0$ in Eq. (21).
The local evaporative heat flux through the liquid microlayer can be determined by Eq. (9), which is a function of the change in pressure across the interface shown in Eq. (12) that has the capillary pressure caused by the curvature. The heat flux profiles for a bubble radius of 0.1mm at various wall superheats can be seen in Figure 10. The heat flux varied greatly depending on wall superheat and radial location. The maximum heat flux for a wall superheat of 2K was about $\sim4.5e5\text{W/m}^2$ at a radial distance of 57.5$\mu$m, while the maximum heat flux for a wall superheat of 8K was about $\sim4.8e6\text{W/m}^2$ at a radial distance of 60.9$\mu$m. The maximum heat flux
flux increased over 10% when the wall superheat was increased by 6K. The heat flux profiles followed a similar trend with a spike in heat flux near the innermost radial coordinate of the microlayer and then a gradual decrease to $R_{\text{max}}$. The heat flux profiles for all wall superheats were zero as the microlayer profile approached its equilibrium thickness near $R_0$, which appeared to be shifted. Also, the calculated heat flux profiles in this under predicted the maximum heat flux in the spike compared to Christopher et al. (2010). Once again, this can be due to the rapid change in magnitude of the parameters as the integration neared the boundary conditions at $R_0$.

Figure 10 – Heat Flux Profiles at a Bubble Radius of 0.1mm
The temperature of the liquid vapor interface can be determined by Eq. (14), which is a function of Fourier’s law, the evaporative heat flux, and the pressure change across the interface. Figure 11 displays the interface temperature along the radial distance of the microlayer. From the heat flux profiles in Figure 10, the zero heat near the equilibrium microlayer radial distance corresponded to where the interface temperature matches the wall temperature. Each wall superheat displayed a linear decrease in the interface temperature; however, the temperature drop became more rapid at higher wall superheat due to the higher amount of heat transfer associated at the higher wall superheats. The total heat transfer rate for a single microlayer profile at a specific wall superheat can be obtained from the integration of Eq. (23) from $R_0$ to $R_{\text{max}}$. 
Figure 11 – Interface Temperature Profiles at a Bubble Radius of 0.1mm

Figure 12 displays the total heat transfer rate for a bubble radius of 0.1mm and 0.5mm at various wall superheats. The total heat transfer rate for a bubble of radius 0.1mm showed a slight concave profile compared to the bubble with a radius of 0.5mm. The total heat transfer rate increased more dramatically for a bubble with a radius of 0.5mm than a bubble with a radius of 0.1mm as the wall superheat increased. The graph also shows that the difference in the total heat transfer rate for the two bubble radii increased with the wall superheat. The total heat transfer rates determined from Christopher et al. (2010) that show comparable results.
Due to the transient nature of the microlayer characteristics during nucleate boiling, the microlayer, heat flux, interface temperature, and total heat transfer profiles were calculated for multiple bubble radii for a given wall superheat. Figure 13 displays the total heat transfer rates at multiple bubble radii for various wall superheats. As the bubble radius increased for a given wall superheat, the total heat transfer rate increased linearly. As the wall superheat increased, the slope also increased. The slope seemed to increase in a relatively constant manner at wall superheats of 4K, 6K, and 8K; however, there appeared to be a larger increase in the slope from
a wall superheat of 2K to 4K. In order to apply the total heat transfer from the microlayer to the growth of the bubble, a linear trend line was determined for each wall superheat from Figure 13. The total heat transfer rate for a given wall superheat as a function of bubble radius can be seen from Eq. (24). The results of the linear trend line of the total heat transfer rate as a function of bubble radius are shown in Table 3 for various wall superheats. In order to keep the total heat transfer rate positive at low bubble radii, a linear trend line was determined from a bubble radius of 0mm to 0.1mm. For a given wall superheat, the total heat transfer rate would follow the linear trend from 0mm to 0.1mm and then follow the equations in Table 3 for the rest of the simulation.
Figure 13 – Total Heat Transfer at Multiple Bubble Radii

Table 3 – Microlayer Total Heat Transfer Equations

<table>
<thead>
<tr>
<th>Wall Superheat: K</th>
<th>$Q_{ml}$: W</th>
</tr>
</thead>
<tbody>
<tr>
<td>2 (375.15K)</td>
<td>$Q_{ml} = 9.3108R_b - 0.0003$</td>
</tr>
<tr>
<td>4 (377.15K)</td>
<td>$Q_{ml} = 14.769R_b - 0.0004$</td>
</tr>
<tr>
<td>6 (379.15K)</td>
<td>$Q_{ml} = 18.210R_b - 0.0003$</td>
</tr>
<tr>
<td>8 (381.15K)</td>
<td>$Q_{ml} = 21.798R_b - 0.0002$</td>
</tr>
</tbody>
</table>
4.3 Single Bubble Simulations

4.3.1 Pure Water

Single vapor bubble simulations in saturated pure water were conducted at two wall superheats of 4K and 8K that applied the phase change model due to the heat transfer from the surrounding liquid and the evaporation of the microlayer as volumetric source terms. The temperature of the liquid vapor interface was held constant at the saturation temperature of 373.15K. The simulations followed similar vapor bubble growth cycles as follows:

1. Initialized as a hemispherical vapor bubble equal to the cavity diameter (see Figure 8)
2. Triple point advanced on the base wall away from the cavity; bubble began to elongate
3. Advancing triple point came to a halt; bubble continued to elongate
4. Triple point receded back on the base wall to the cavity; bubble continued to elongate
5. Triple point reached the cavity edge and began necking
6. Necking continued until the bubble departed and then ascended
7. A new bubble formed on the cavity and the growth cycle process repeated itself

The saturated water properties at 373.15K that were used in this study can be seen in Table 1. The cavity diameter was chosen to be 60µm in order to capture the necking process of the bubble near the end of its growth cycle. According to the results by Mukherjee et al. (2007), a static contact angle can be used in the absence of experimental data, and 38° was the chosen to match the microlayer characteristics that were determined in Section 4.1. The departure time for each simulation was divided into five non-dimensional time segments for growth comparisons.

The vapor and temperature profiles for pure water at a wall superheat of 4K are displayed in Figure 14. The departure time came to be 155.54ms at a volume of 5.793mm³. The bubble
was treated as a sphere in order to calculate the departing diameter of 2.23mm. The temperature contour legend for a wall superheat of 4K can be found in the enlarged departing profiles in Figure 15. From the temperature contours, the heat transfer from the superheated wall conducted through the liquid and also the vapor bubble. The heat transfer in the vapor conducted faster than in the liquid due to the difference in properties. Inside the bubble, the temperature of the vapor became layered and conducted more heat into the bubble as it advances along the base wall due to the increases vapor surface area on the superheated wall. As the bubble receded towards the cavity, the vapor area in contact with the superheated wall became less. The vapor became only slightly higher than the saturation temperature at departure. The temperature contours also displayed the movement of the liquid surround the bubble. As the vapor bubble began to advance, the interface pushed the surrounding superheated liquid up along the interface creating a small wake. When the triple contact point receded, an eddy pocket was beginning to form along the superheated wall and the interface. The eddy development can be seen in the five non-dimensional time segments in Figure 14 and Figure 15 shows the fully developed eddy. The formation of the eddy indicated another heat transfer mechanism due to convection (not applied).

| Pure Water Vol | 0.562mm³ | 1.700mm³ | 2.917mm³ | 4.407mm³ | 5.793mm³ |
| Pure Water Dia | 1.02mm | 1.48mm | 1.77mm | 2.03mm | 2.23mm |
| t/tₐ | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |

Figure 14 – Profiles for Pure Water at a Wall Superheat of 4K (Tₜ = 377.15K)
Similar to the wall superheat of 4K study, a simulation at 8K was completed and compared. The results at the wall superheat of 8K are displayed in Figure 16. The temperature contour legend for a wall superheat of 8K can be found in the enlarged departing profiles in Figure 17. The departure time for this simulation came to be 126.53ms at a volume of 6.884mm$^3$.
and a diameter of 2.36mm. The temperature contours inside the vapor bubble displayed a similar layered pattern the 4K wall superheat simulation. The liquid surrounding the vapor bubble did form a wake and an eddy as the triple contact point advanced along the base wall. From the temperature profiles in Figure 16, the eddy detached from the interface as the triple contact point receded toward the cavity. This could be possible due to the rate change at which the triple contact point advanced and receded along the base wall. Figure 17 shows the fully developed eddy can be seen as detached from the liquid vapor interface. Convection appeared to be a stronger contributor as the eddy was developing and attached to interface during the earlier growth stages of the vapor bubble.

![Figure 16](image1)

<table>
<thead>
<tr>
<th>Pure Water Vol</th>
<th>0.814mm³</th>
<th>2.201mm³</th>
<th>3.600mm³</th>
<th>5.201mm³</th>
<th>6.884mm³</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pure Water Dia</td>
<td>1.16mm</td>
<td>1.61mm</td>
<td>1.90mm</td>
<td>2.15mm</td>
<td>2.36mm</td>
</tr>
<tr>
<td>t/tₜ</td>
<td>0.2</td>
<td>0.4</td>
<td>0.6</td>
<td>0.8</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Figure 16 – Profiles for Pure Water at a Wall Superheat of 8K (Tₜ = 381.15K)
Figure 17 – Pure Water Departing Temperature Profile at a Wall Superheat of 8K

The comparison of the vapor bubble profiles at the same non-dimensional time in pure water is displayed in Figure 18. Figure 19 displays the volume growth rates where the departure time for the wall superheat of 4K was applied to non-dimensionalize the time intervals for the wall superheat of 8K. The wall superheat of 8K grew faster due to the higher heat transfer rates...
from the superheated wall and microlayer. The departure time for the wall superheat of 8K was 81.3% of 4K. The departing volume for the vapor bubble at a wall superheat of 4K was 5.793mm$^3$ at a time of 155.54ms and at 8K was 6.884mm$^3$ a time of 126.53ms. Similar trends were noticed by Abarajith et al. (2002), who numerically simulated multiple contact angles for a variety of wall superheats. The results for a constant contact angle and various wall superheats concluded that the departure diameter became greater as the wall superheat increased while the time period of growth decreased.

<table>
<thead>
<tr>
<th>$\Delta T_w = 4K$</th>
<th>$\Delta T_w = 8K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta = 38^\circ$</td>
<td>$\theta = 38^\circ$</td>
</tr>
<tr>
<td>$t_d = 155.54ms$</td>
<td>$t_d = 126.53ms$</td>
</tr>
<tr>
<td>$t_d = 81.3%$ of 4K</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>4K Pure Water Vol</th>
<th>8K Pure Water Vol</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.562mm$^3$</td>
<td>0.814mm$^3$</td>
</tr>
<tr>
<td>1.700mm$^3$</td>
<td>2.201mm$^3$</td>
</tr>
<tr>
<td>2.917mm$^3$</td>
<td>3.600mm$^3$</td>
</tr>
<tr>
<td>4.407mm$^3$</td>
<td>5.201mm$^3$</td>
</tr>
<tr>
<td>5.793mm$^3$</td>
<td>6.884mm$^3$</td>
</tr>
</tbody>
</table>

| $t/t_d$ | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |

Figure 18 – Vapor Profiles in Pure Water
Figure 19 – Vapor Volume Growth Rate in Pure Water
4.3.2 Surfactants

Surfactant is a name for a surface-active agent. Surfactants adsorb at surfaces and interfaces when applied to an aqueous solution in low concentrations. Surfactants are typically made up of two sections consisting of a hydrophobic tail, which is a long chain hydrocarbon, and a hydrophilic head, which is ionizable, polarizable, and suitable for making hydrogen bridges as shown in Figure 20.

![Typical Surfactant Molecule](Deodhar et al. (2012))

Figure 20 – Surfactant Molecule Composition [Deodhar et al. (2012)]

When a surfactant is dissolved in water, they align themselves at the interface such that the hydrophobic tail points toward the vapor and the hydrophilic head points toward the liquid. Surfactants are classified depending on the nature of the hydrophilic head group as follows:

1. Anionic: Surface active section has a negative charge
2. Cationic: Surface active section has a positive charge
3. Nonionic: Surface active section has no apparent ionic charge
4. Zwitterionic: Surface action section may have both positive and negative charge

As the surfactant is adsorbed at the interface, the surface tension of the solution reduces. The surface tension will continue to decrease with the increase in concentration until the Critical Micelle Concentration (CMC) is reached, beyond which the surface tension remains at an
equilibrium value. This time-dependent process of adsorption-desorption results in a dynamic surface tension behavior as illustrated in Figure 21.

![Dynamic Surface Tension for Aqueous Surfactants](image)

**Figure 21 – Dynamic Surface Tension for Aqueous Surfactants [Deodhar et al. (2012)]**

Surface wettability or contact angle is directly related to surface tension in the spreading of a liquid on a solid surface by an expression known as Young’s equation:

\[
\sigma_{SG} = \sigma_{SL} + \sigma_{LG} \cos \theta
\]  \hspace{1cm} (46)

The force balance in Eq. (46) contains the liquid-gas, \( \sigma_{LG} \), solid-gas, \( \sigma_{SG} \), and solid-liquid, \( \sigma_{SL} \), interfacial surface tensions. Their interactions at the triple contact point can be seen in Figure 22. Dynamic surface tension and contact angle play a critical role in nucleate boiling by changing the force balance on the vapor bubble during its growth cycle.
In this boiling study, three surfactants were considered: sodium dodecyl sulfate (SDS: anionic), cetyltrimethylammonium bromide (CTAB: cationic), and octylphenol ethoxylate (Triton X-100: nonionic). Wasekar et al. (2001) and Zhang et al. (2004) experimentally determined the dynamic surface tension profiles at 296.15K (23°C) and the equilibrium surface tension at 353.15K (80°C) for the three surfactants. Figure 23 displays two sets of surface tension profiles with respect to time. The first set contains data at concentrations of 2×CMC where each surfactant solution begins at the surface tension of pure water at 296.15K, 72.1mN/m, and ends at their respective equilibrium surface tension value. The second set was normalized with respect to the first set where each surfactant profile starts at the surface tension of pure water at 353.15K, 62.6mN/m, follows a similar shape as the first set, and then ends at the measured equilibrium surface tension, which was 34.4mN/m for SDS, 28.7mN/m for Triton X-100, and 34.7mN/m for CTAB. The profiles of the second set were extrapolated to create a boiling set that starts at the surface tension of pure water at 373.15K (100°C), 58.9mN/m, and ends at an equilibrium surface tension slightly below the measurements at 353.15K. Extending the dynamic surface tension profiles in Figure 23 would end at each surfactant’s equilibrium surface tension value like the profile in Figure 21. Each surfactant’s dynamic surface tension profile is dependent on their adsorption/desorption rate, CMC value, and molecular weight. A
surfactant with a lower molecular weight (SDS) will adsorb faster than one with a higher molecular weight (CTAB and Triton X-100). Figure 24 shows the contact angle measurements on a steel surface at room temperature of 296.15K based on the surfactant concentration by Zhang et al. (2004). For all surfactant solutions, the contact angle decreased with an increase in surfactant concentration and then plateaued at their respective equilibrium contact angle. SDS and CTAB plateaued near their respective CMC values; Triton X-100 met its equilibrium contact angle prior to reaching its CMC value due to molecular characteristics of nonionic surfactants.

![Dynamic Surface Tension Profiles](image)

Figure 23 – Dynamic Surface Tension Profiles [Wasekar et al. (2001) & Zhang et al. (2004)]
Figure 24 – Contact Angle Measurements on Steel [Zhang et al. (2004)]
Single vapor bubble simulations were conducted for all three surfactants at a wall superheat of 4K, only SDS was simulated for a wall superheat of 8K. Similar to the pure water simulations, the temperature of the liquid vapor interface was held constant at the saturation temperature of 373.15K, and the cavity diameter was kept at 60µm. A six order polynomial curve fit was applied to the boiling dynamic surface tension profiles for each surfactant in Figure 23 allowing the simulation to change the surface tension with respect to time. Table 4 displays the equilibrium contact angles determined at 2×CMC from Figure 24 with a pure water static contact angle of 38°. Each surfactant simulation had a static contact angle throughout the simulation like in the pure water cases. The surfactant simulations assume that the surface tension over the interface for a given time is constant. Due to the high concentration of the solutions at 2×CMC, the liquid-vapor interface is stretched and surfactant molecules from micelle structures can be quickly adsorbed on the interface. This process is likely to maintain uniform surfactant concentration along the interface compared to low bulk concentrations where surfactant molecules will slowly diffuse from the bulk liquid to any newly created interface.

<table>
<thead>
<tr>
<th>Solution</th>
<th>Contact Angle, ( \theta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>SDS</td>
<td>( \theta = 17.5^\circ )</td>
</tr>
<tr>
<td>CTAB</td>
<td>( \theta = 29.5^\circ )</td>
</tr>
<tr>
<td>Triton X-100</td>
<td>( \theta = 20^\circ )</td>
</tr>
</tbody>
</table>

The vapor and temperature profiles for SDS solution at a wall superheat of 4K are displayed in Figure 25. The temperature contour legend is the same used in Figure 15. The departure time of the SDS vapor bubble came to be 66.88ms at a volume of 1.003mm\(^3\) and a diameter of 1.24mm. Unlike the pure water growth cycle, the SDS growth cycle did not have the triple contact point advance on the base wall. Due to the triple contact point being pinned at the
edge of the cavity, the cavity superheated surface was the only section of the wall able to conduct heat into the vapor keeping the temperature inside of the bubble at the saturation temperature of 373.15K. Similar to the trends seen in the pure water simulations, the growing bubble pushed the surrounding superheated liquid up along the interface creating a small wake. Since the triple contact point did not advance, an eddy was unable to form.

<table>
<thead>
<tr>
<th>SDS: 2×CMC</th>
<th>( \theta = 17.5^\circ )</th>
<th>( t_d = 66.88 \text{ms} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>SDS Vol</td>
<td>0.123mm(^3)</td>
<td>0.345mm(^3)</td>
</tr>
<tr>
<td>SDS Dia</td>
<td>0.62mm</td>
<td>0.87mm</td>
</tr>
<tr>
<td>( t/t_d )</td>
<td>0.2</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Figure 25 – Profiles for SDS Solution at a Wall Superheat of 4K (\( T_w = 377.15 \text{K} \))

The vapor and temperature profiles for Triton X-100 solution at a wall superheat of 4K are displayed in Figure 26. The temperature contour legend is the same used in Figure 15. The departure time of the Triton X-100 vapor bubble came to be 56.11ms at a volume of 0.999mm\(^3\) and a diameter of 1.24mm. The triple contact point did advance off the cavity edge a very small amount. This was easily noticed in the small layered temperature contours inside the bubble. Similar to the trend seen in the previous simulation of the SDS solution at a wall superheat of 4K, the triple contact point did not advance enough to create an eddy. Also, the temperature contours outside the growing vapor bubble showed the superheated liquid getting pushed up along the interface creating a small wake.
The vapor and temperature profiles for CTAB at a wall superheat of 4K are displayed in Figure 27. The temperature contour legend is the same used in Figure 15. The departure time of the CTAB vapor bubble came to be 73.80 ms at a volume of 1.948 mm$^3$ and a diameter of 1.55 mm. From the profiles, CTAB followed the growth cycles of the pure water simulations by advancing and receding on the base wall. Inside the bubble, the layered temperature bands were seen. As the bubble advanced, the growing bubble pushed the surrounding superheated liquid up along the interface. An eddy did begin to form as the triple contact point receded toward the cavity; however, as the vapor bubble departed, the eddy was detached from the liquid vapor interface, what was similar to the trends seen in the simulation of pure water at a wall superheat of 8K. Again, the change in the rates at which the triple contact point advanced and receded along the base wall could be responsible for the eddy detachment from the interface.
The vapor profiles for the pure water and three surfactant simulations at a wall superheat of 4K are displayed in Figure 28, and their respective volume growth rates using non-dimensional time are graphed in Figure 29. The volume growth rates in Figure 29 used the departure time of pure water to non-dimensionalize the time intervals for the surfactants. The pure water simulation had the longest growth time with the largest departing volume. The departing volume and time for the three surfactants was much less than pure water due to the dynamic surface tension and reduced equilibrium contact angle. The departure time for SDS came to be 43.0% of pure water, while Triton X-100 and CTAB came to be 36.1% and 47.4% of pure water, respectively. SDS and Triton X-100 had similar departing volumes; however, the departure time for Triton X-100 was lower than SDS even though SDS has a lower contact angle. The simulated boiling results by Abarajith et al. (2002) showed that as the constant contact angle was decreased for a given wall superheat, the departure time and diameter decreased, which was consistent with other researchers in two phase flow. Triton X-100 departed faster than SDS due to two possibilities: the small advancement of the triple contact point on the base wall shifting liquid at a greater rate and its dynamic tension profile. Figure 23
shows that the surface tension profile for SDS initially decreased faster than Triton X-100. At around 70ms, the surface tension of Triton X-100 dropped below SDS. Even though both of these simulations departed before the cross, the slope of SDS prior to this point reduced as the slope of Triton X-100 became steeper changing the force balance on the bubble. CTAB has a much higher contact angle than both SDS and Triton X-100. The dynamic surface tension profile initially followed the profile of Triton X-100, and then followed SDS after the point where Triton X-100 dropped below SDS. Due to these two descriptions of CTAB, the departure volume and time was longer than SDS and Triton X-100, but less than pure water.

<table>
<thead>
<tr>
<th></th>
<th>Pure Water</th>
<th>SDS: 2×CMC</th>
<th>Triton X-100: 2×CMC</th>
<th>CTAB: 2×CMC</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \theta = 38^\circ )</td>
<td>( \theta = 17.5^\circ )</td>
<td>( \theta = 20.0^\circ )</td>
<td>( \theta = 29.5^\circ )</td>
<td></td>
</tr>
<tr>
<td>( t_d = 155.54 \text{ms} )</td>
<td>( t_d = 66.88 \text{ms} )</td>
<td>( t_d = 56.11 \text{ms} )</td>
<td>( t_d = 73.80 \text{ms} )</td>
<td></td>
</tr>
<tr>
<td>( t_d = 43.0% \text{ of pw} )</td>
<td>( t_d = 43.0% \text{ of pw} )</td>
<td>( t_d = 36.1% \text{ of pw} )</td>
<td>( t_d = 47.4% \text{ of pw} )</td>
<td></td>
</tr>
<tr>
<td>Pure Water Vol</td>
<td>0.562mm(^3)</td>
<td>0.123mm(^3)</td>
<td>0.104mm(^3)</td>
<td>0.171mm(^3)</td>
</tr>
<tr>
<td>1.700mm(^3)</td>
<td>0.345mm(^3)</td>
<td>0.325mm(^3)</td>
<td>0.503mm(^3)</td>
<td>0.516mm(^3)</td>
</tr>
<tr>
<td>2.917mm(^3)</td>
<td>0.562mm(^3)</td>
<td>0.560mm(^3)</td>
<td>0.965mm(^3)</td>
<td>0.965mm(^3)</td>
</tr>
<tr>
<td>4.407mm(^3)</td>
<td>0.786mm(^3)</td>
<td>0.794mm(^3)</td>
<td>1.485mm(^3)</td>
<td>1.485mm(^3)</td>
</tr>
<tr>
<td>5.793mm(^3)</td>
<td>1.002mm(^3)</td>
<td>0.999mm(^3)</td>
<td>1.948mm(^3)</td>
<td>1.948mm(^3)</td>
</tr>
</tbody>
</table>

| \( t/t_d \)        | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 |

Figure 28 – Vapor Profiles at a Wall Superheat of 4K \( (T_w = 377.15K) \)
The vapor and temperature profiles for SDS solution at a wall superheat of 8K are displayed in Figure 30. The temperature contour legend is the same used in Figure 17. The departure time of the SDS vapor bubble came to be 47.50ms at a volume of 1.262mm$^3$ and a diameter of 1.34mm. From the profiles, the triple contact point advanced off the cavity edge a fairly small amount, but not enough to where an eddy was able to fully form. Similar to the trends seen in the simulation results of pure water at a wall superheat of 8K and CTAB at 4K, the
superheated liquid detached from the liquid vapor interface as the triple contact point receded due to the rate change at which the triple contact point advanced and receded along the base wall.

<table>
<thead>
<tr>
<th>SDS: 2×CMC</th>
<th>( \theta = 17.5^\circ )</th>
<th>( t_d = 47.50)ms</th>
</tr>
</thead>
<tbody>
<tr>
<td>SDS Vol</td>
<td>0.167mm(^3)</td>
<td>0.444mm(^3)</td>
</tr>
<tr>
<td>SDS Dia</td>
<td>0.68mm</td>
<td>0.95mm</td>
</tr>
<tr>
<td>( t/t_d )</td>
<td>0.2</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Figure 30 – Profiles for SDS Solution at a Wall Superheat of 8K (\( T_w = 381.15K \))

The vapor profiles for the pure water and the SDS solution simulations at a wall superheat of 8K are displayed in Figure 31, and their respective volume growth rates using non-dimensional time are graphed in Figure 32. The volume growth rates in Figure 32 used the departure time of pure water to non-dimensionalize the time intervals for the surfactant. The departure time for SDS came to be 37.5% of pure water. Similar to the trends seen in the simulation results at a wall superheat of 4K, the pure water simulation had the longest growth time at 126.53ms with the largest departing volume of 6.884mm\(^3\) and SDS had a much smaller departing volume of 1.262mm\(^3\) and time of 47.50ms.
<table>
<thead>
<tr>
<th>Pure Water</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\theta = 38^\circ$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t_d = 126.53$ ms</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pure Water Vol</td>
<td>0.814mm$^3$</td>
<td>2.201mm$^3$</td>
<td>3.600mm$^3$</td>
<td>5.201mm$^3$</td>
<td>6.884mm$^3$</td>
</tr>
<tr>
<td>SDS: 2xCMC</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\theta = 17.5^\circ$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t_d = 47.50$ ms</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$t_d = 37.5%$ of pw</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SDS Vol</td>
<td>0.167mm$^3$</td>
<td>0.444mm$^3$</td>
<td>0.725mm$^3$</td>
<td>0.996mm$^3$</td>
<td>1.262mm$^3$</td>
</tr>
<tr>
<td>$t/t_d$</td>
<td>0.2</td>
<td>0.4</td>
<td>0.6</td>
<td>0.8</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Figure 31 – Vapor Profiles at a Wall Superheat of 8K ($T_w = 381.15$K)
Figure 32 – Vapor Volume Growth Rate at a Wall Superheat of 8K ($T_w = 381.15K$)

The comparison of the vapor bubble profiles at the same non-dimensional time in SDS solution is displayed in Figure 33, and the volume growth rate is graphed in Figure 34. Figure 34 displays the volume growth rates where the departure time for the wall superheat of 4K was applied to non-dimensionalize the time intervals for the wall superheat of 8K. The departure time for the wall superheat of 8K was 71.0% of 4K. The departing volume for the vapor bubble at a wall superheat of 4K was 1.002mm$^3$ at a time of 66.88ms and at 8K was 1.262mm$^3$ at a time of 47.50ms. Similar to the trend seen in the pure water comparison, the wall superheat of 8K
grew faster due to the higher heat transfer rates from the wall superheat and microlayer leading to a faster departure time. The departing volume for the vapor bubble at a wall superheat of 8K was higher than 4K following the same trend that was seen in the pure water comparison.

<table>
<thead>
<tr>
<th>$\Delta T_w = 4K$</th>
<th>$\theta = 17.5^\circ$</th>
<th>$t_d = 66.88$ms</th>
</tr>
</thead>
<tbody>
<tr>
<td>4K SDS Vol</td>
<td>0.123mm$^3$</td>
<td>0.345mm$^3$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$\Delta T_w = 8K$</th>
<th>$\theta = 17.5^\circ$</th>
<th>$t_d = 47.50$ms</th>
<th>$t_d = 71.0%$ of 4K</th>
</tr>
</thead>
<tbody>
<tr>
<td>8K SDS Vol</td>
<td>0.167mm$^3$</td>
<td>0.444mm$^3$</td>
<td>0.725mm$^3$</td>
</tr>
<tr>
<td>$t/t_d$</td>
<td>0.2</td>
<td>0.4</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Figure 33 – Vapor Profiles in SDS Solution (2×CMC)
Figure 34 – Vapor Volume Growth Rate in SDS Solution (2×CMC)
CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

5.1 Conclusions

Nucleate pool boiling for pure water and 2×CMC concentrated surfactant solutions were computationally modeled from incipience to departure using the Volume-of-Fluid (VOF) method. Vapor generation due to evaporation of the microlayer and phase change in the superheated liquid layer was represented as source terms in the macro region governing equations. The equations that govern the microlayer were solved for a variety of superheats at multiple bubble radii comparing well with the results available in literature. The pure water simulations included wall superheats of 4K and 8K. The wall superheat of 8K had a faster growth rate leading to a faster departure time and a higher departure volume due to the higher heat transfer rates from the evaporation of the microlayer and wall superheat. The predictions of the departure diameter and growth rate with increasing wall superheat agree well with the results available in literature.

Three surfactants were considered: sodium dodecyl sulfate (SDS), cetyltrimethylammonium bromide (CTAB), and octylphenol ethoxylate (Triton X-100). The dynamic surface tension profiles and the contact angles for the three surfactants at a concentration of 2×CMC were determined using experimental data from Zhang et al. (2004). For a wall superheat of 4K, the departing volume and time for the three surfactants was much less than pure water due to the dynamic surface tension and reduced equilibrium contact angle. SDS and Triton X-100 had similar growth rates and departing volume, but the departure time for Triton X-100 was lower than SDS due to their respective dynamic surface tension profiles. CTAB has a higher equilibrium contact angle than SDS and Triton X-100. Due to its dynamic
surface tension profile and contact angle, the departure volume and time of CTAB was larger than SDS and Triton X-100, but less than pure water. For a wall superheat of 8K, only SDS was simulated for a comparison to pure water. Pure water had a longer growth time and larger departing volume than SDS. The SDS simulation results at different wall superheats showed a similar trend to pure water where the wall superheat of 8K grew faster and had a larger departing volume than 4K.

The goal to increase thermal efficiency requires a solution to remove as much heat from the surface as possible in the shortest amount of time. The best solution is one where the bubble grows at the fastest rate having the smallest departure time. The faster the bubble departs, the faster the surface is rewetted to begin the boiling cycle again. This removes heat from the surface more frequently than bubbles that take a long time grow and depart. The higher the bubble departure frequency, the higher the heat transfer is from the surface increasing the thermal efficiency. This study shows that surfactant solutions produce smaller departure volume of bubbles that detach at higher frequency than those formed in pool boiling of pure water. Surfactants provide a passive method of heat transfer enhancement in pool boiling.

5.2 Recommendations for Future Work

This study showed the computation results for pure water and three surfactant solutions during nucleate pooling boiling. For the surfactant simulations, a more in depth adsorption-desorption model can be implemented. Additional surfactant and even polymer solutions can be investigated to provide a better understanding of surface tension and wettability characteristics in nucleate pool boiling. An improved adsorption-desorption model would allow for non-
uniformity of surfactant concentration along the interface. This may lead to Maragoni convection, which could be investigated.

In the conducted simulations, the contact angle was kept constant when in nature the contact angle tends to vary as the vapor bubble advances and recedes along the base wall. Computational simulations involving multiple wall superheats, contact angles, and cavity diameters can provide useful insight to nucleate pool boiling characteristics.

Comparing the simulations conducted in this study to experimental data is challenging due to complications with keeping the surface at a constant wall temperature during the experiment. A known heat flux is generally used to heat the surface during experimental nucleate boiling. If a thick wall of highly conductive material (for example, copper) is used in the experiments, the wall temperature is likely to be nearly uniform when a constant heat flux is applied. A conjugate analysis of conduction through the wall and pool boiling from the wall surface can be performed to compare the results of a constant-wall simulation with experimental measurements.
REFERENCES


