Thesis

Presented to the University of Cergy Pontoise in partial fulfillment of the degree requirements for the
degree of Doctor of Philosophy in Civil Engineering

by:

Muhammad Sajid

A contribution towards the numerical study of bubble dynamics in nucleate boiling at local scale
using a conservative level set method

Defended on 27 August 2010, with the jury:

Dr. Bernard PATEYRON,     Univ. of Limoges       Reporter
Pr. Hamou SADAT,            Univ. of Poitiers      Reporter
Pr. Khelil SEFIANE,         Univ. of Edinburgh     Examiner
Dr. Adrien BOUVET,          Univ. of Cergy-Pontoise Examiner
Pr. Rachid BENNACER,        Univ. of Cergy-Pontoise Supervisor

Laboratoire de Mécanique et Matériaux de Genie Civil. L2MGC-EA 4114
University of Cergy Pontoise

© Sajid 2010
Abstract

1. English
A contribution towards numerical study of bubble dynamics in nucleate boiling at local scale using a conservative level set method.

Nucleate boiling is an efficient means of heat transfer that has been the subject of many studies which have lead to more empirical results than knowledge on the physical mechanisms that govern the phenomena. In this work, a conservative level set method (LSM) was applied to the study of bubble dynamics during nucleate pool boiling which reduces the computational cost of reinitialization techniques traditionally used with LSM to limit phase loss. Also a force-balance approach to modelling dynamic apparent contact angle (CA) was proposed in this study based on the physics of the moving contact line (CL). It was tested against the traditional CL velocity approach and validated in comparison to available experimental data. In comparison to the CL velocity model our approach reduces the non-physical stick/slip behaviour of the CL and allows a smoother transition from the minimum receding to the maximum advancing CA, which is more akin to the physical phenomena. It was also demonstrated that the heat transfer during bubble growth is proportional to the apparent CA.

2. French
Une contribution à l'étude numérique de la dynamique des bulles en ébullition nucléée à l'échelle locale, en utilisant la méthode 'level set' conservative.

L’ébullition nucléée est un moyen efficace de transfert de chaleur qui a fait l’objet de nombreuses études qui ont conduit vers des résultats davantage empiriques que de connaissances sur les mécanismes physiques qui régissent les phénomènes. Dans ce travail, une méthode 'level-set' (LSM) a été appliquée à l'étude de la dynamique des bulles lors de l’ébullition nucléée. Cette méthode réduit le coût de calcul en comparaison aux précédentes techniques de réinitialisation utilisées avec LSM pour limiter les pertes de masse. Une nouvelle approche, basée sur la physique de la ligne de contact (CL) mobile et le bilan de forces, permet la modélisation de l’angle de contact (CA) apparent dynamique. Elle est comparée avec l'approche classique "vitesse de CL" et validée par rapport aux données expérimentales disponibles. Cette nouvelle approche réduit le comportement non-physique accroche-glissement de CL et permet une transition plus douce entre le minimum et le maximum de CA, ce qui est plus proche des phénomènes physiques observés. Il a également été démontré que le transfert de chaleur au cours de la croissance des bulles est proportionnel à CA apparent.
Acknowledgements

I would like to thank my advisor Professor Rachid Bennacer for his guidance and support during the course of this long study. His frequent encouragement and erudite counsel was invaluable in keeping me on track to complete this work.

I dedicate this work to the pursuit of knowledge, excellence and the realization of dreams and all those that abetted me in my own pursuit, my parents who encouraged me, my mentors who guided me and last but not least the special friends and family members who have always supported me.

I am also grateful for the financial support extended by the Higher Education Commission of the government of Pakistan.
Table of Contents

Abstract........................................................................................................................................ii

Acknowledgements ................................................................................................................iii

Table of Contents ......................................................................................................................iv

List of Figures ..........................................................................................................................vii

List of Tables ............................................................................................................................x

Chapter 1 General introduction.................................................................................................11
  1.1 Outline of the thesis ............................................................................................................13

Chapter 2 Literature review ......................................................................................................14
  2.1 Boiling and boiling curve ....................................................................................................14
     2.1.1 Natural convection regime .......................................................................................17
     2.1.2 Nucleate boiling regime .........................................................................................18
     2.1.3 Film boiling regime (FB) .......................................................................................21
     2.1.4 Transition boiling regime (TB) .............................................................................22
  2.2 Length scales ....................................................................................................................23
     2.2.1 Two phase flow scale .............................................................................................24
     2.2.2 Mean bubble growth scale .....................................................................................25
     2.2.3 Local scale .............................................................................................................26
  2.3 Bubble dynamics ...............................................................................................................27
     2.3.1 Contact angle ..........................................................................................................28
     2.3.2 Nucleation ...............................................................................................................30
     2.3.3 Bubble growth .........................................................................................................32
     2.3.4 Bubble departure .....................................................................................................35
     2.3.5 Bubble release frequency .......................................................................................36
  2.4 Heat transfer mechanisms .................................................................................................38
     2.4.1 Bubble agitation .......................................................................................................38
     2.4.2 Vapor-liquid exchange ...........................................................................................38
     2.4.3 Evaporation .............................................................................................................39
     2.4.4 Heat transfer overview ...........................................................................................41
  2.5 Numerical simulation ........................................................................................................42
4.1.2 Bubble diameter comparison ...................................................................... ........................................96
4.2 Local conditions and bubble growth ............................................................97
  4.2.1 Effects of profile of the interface velocity...............................................98
  4.2.2 Effects of the rate of evaporation ............................................................105
4.3 Conclusions ..................................................................................................108

Chapter 5 Coupled bubble dynamics .................................................................109
  5.1 Bubble growing on heated surface ..............................................................109
    5.1.1 Evolution of the temperature field .......................................................110
    5.1.2 Progression of the flow field ...............................................................113
    5.1.3 Heat transfer .......................................................................................114
    5.1.4 Phase conservation ............................................................................116
  5.2 Dynamic contact angle ..............................................................................118
    5.2.1 Case-I: static contact angle ...............................................................119
    5.2.2 Case-II: Contact line velocity approach .............................................120
    5.2.3 Case-III: Force balance approach .....................................................124
    5.2.4 Comparison with experimental data ...................................................124
    5.2.5 Heat transfer comparison .................................................................127
  5.3 Conclusion ..................................................................................................129

Chapter 6 Concluding remarks ........................................................................130
  6.1 Advances made in this work .................................................................130
  6.2 Publications during PhD studies ..............................................................131
  6.3 Outlook .....................................................................................................132

Bibliography .....................................................................................................133

Appendix A Comsol scripting code ................................................................139
List of Figures

Figure 2.1: Temperature distribution in pool boiling ............................................................... 15
Figure 2.2: The Nukiyama boiling curve for saturated water. Adapted from Incropera and DeWitt (2006) using the data of Nukiyama (1934) ............................................................... 16
Figure 2.3: Characteristics of the boiling curve for a heated horizontal surface ....................... 17
Figure 2.4: Natural Convection ......................................................................................... 18
Figure 2.5: Onset of nucleate boiling ................................................................................ 18
Figure 2.6: Low heat flux nucleate boiling .......................................................................... 19
Figure 2.7: High heat flux nucleate boiling .......................................................................... 20
Figure 2.8: Critical heat flux (CHF) .................................................................................. 20
Figure 2.9: Film boiling regime (FB) ................................................................................ 22
Figure 2.10: Transition Boiling Regime ............................................................................. 23
Figure 2.11: The length scales of description of nucleate boiling, (a) Two phase flow scale (b) Mean bubble growth scale and (c) Local scale ........................................................................ 24
Figure 2.12: Bubble growth model of van Stralen (1966) ................................................... 35
Figure 2.13: Bubble agitation ............................................................................................ 38
Figure 2.14: Vapor-liquid heat exchange .......................................................................... 39
Figure 2.15: Evaporation .................................................................................................. 40
Figure 2.16: Explicit and implicit interface representation ................................................... 43
Figure 2.17: ALE Grid ...................................................................................................... 45
Figure 2.18: FTM Grid ..................................................................................................... 45
Figure 3.1: Heaviside Function, smooth Heaviside function and delta function ................. 52
Figure 3.2: Surface plot of the unit circle centred at origin at t=0 with the level set function as (a) a distance function, (b) a Heaviside function, and as (c) a hyperbolic tangent function ...... 54
Figure 3.3: Advancing and receding contact angles of n-Alkanes and 1-Alcohols versus the mean contact angle, $\theta_0$. Data from Lam \textit{et al.}(2002) ........................................ 63
Figure 3.4: Characteristic experimental results for contact angle measurements against contact line velocity. .................................................................64
Figure 3.5: Navier-Slip boundary condition .....................................................................................69
Figure 3.6: Computational domain ..................................................................................................74
Figure 3.7: Relaxation of an elliptical vapor bubble of aspect ratio of 2:1 at various times with a vector plot of surface tension forces ..................................................................................80
Figure 3.8: Relaxation of an elliptical vapor bubble of aspect ratio of 7:4 at various times with a vector plot of surface tension forces ..................................................................................81
Figure 3.9: Relaxation of an elliptical vapor bubble of aspect ratio of 3:2 at various times with a vector plot of surface tension forces ..................................................................................82
Figure 3.10: Relative error in area of vapor phase .............................................................................83
Figure 3.11: Relative error in area of vapor phase for the three aspect ratios ........................................84
Figure 3.12: Area of the vapor phase for the three aspect ratios ..........................................................85
Figure 3.13: Relative error in area of vapor phase for various mesh densities ...............................................86
Figure 3.14: Initial state of the domain ................................................................................................87
Figure 3.15: Phase loss during initialization of the level set function ..................................................88
Figure 3.16: Coalescence of two bubbles ............................................................................................88
Figure 3.17: Phase loss during coalescence ..........................................................................................89
Figure 4.1: Profile of the injected velocity ............................................................................................92
Figure 4.2: Bubble base diameter for contact angle, $\theta_{CA} = 50^\circ$, $\theta_{CA} = 55^\circ$ and $\theta_{CA} = 60^\circ$ .................................................................93
Figure 4.3: Equivalent bubble diameter for contact angle, $\theta_{CA} = 50^\circ$, $\theta_{CA} = 55^\circ$ and $\theta_{CA} = 60^\circ$. .................................................................94
Figure 4.4: Equivalent bubble departure diameter calculated and computed from empirical relations. ..............................................................................................................................97
Figure 4.5: Height of velocity profiles, $h_u$ .........................................................................................100
Figure 4.6: Velocity profiles, $u_{exp}$ for $\alpha=3,2,1,0.5$ and 0.33 at time = 3 ........................................101
Figure 4.7: Rate of vapor injection, $\dot{V}$ ..........................................................................................102
Figure 4.8: Non dimensional volume of vapor bubble ..........................................................................103
Figure 4.9: Equivalent bubble diameter for various $\alpha$’s at $\theta_{CA} = 52^\circ$ ........................................................ 104
Figure 4.10: Bubble base diameter for various $\alpha$’s at $\theta_{CA} = 52^\circ$ ........................................................ 105
Figure 4.11: Velocity profiles, $u_{exp}$ for $\dot{\alpha} = 1/2$ and $2/3$ at time = 3.5 ........................................................ 106
Figure 4.12: Bubble base diameter for $\dot{\alpha} = 1/2$ and $\dot{\alpha} = 2/3$ at $\theta_{CA} = 52^\circ$ ................................................ 107
Figure 4.13: Volume of vapour bubble for $\dot{\alpha} = 1/2$ and $\dot{\alpha} = 2/3$ at $\theta_{CA} = 52^\circ$ ................................................ 107
Figure 5.1: Temperature field (in K) at $t = 0$s ........................................................ 110
Figure 5.2: Temperature field (in K) at $t = 0.01$s ........................................................ 111
Figure 5.3: Temperature field (in K) at $t = 0.11$s ........................................................ 111
Figure 5.4: Temperature field (in K) at $t = 0.14$s ........................................................ 112
Figure 5.5: Temperature field (in K) at $t = 0.16$s ........................................................ 112
Figure 5.6: Normalized flow field at $t = 0.0s$, $0.01$s and $0.11$s ................................................ 113
Figure 5.7: Normalized flow field at $t = 0.0s$, $0.01$s and $0.11$s ................................................ 114
Figure 5.8: Latent heat flux from a growing bubble ........................................................ 115
Figure 5.9: Total heat absorbed by vapor bubble ........................................................ 116
Figure 5.10: Phase conservation during simulation ........................................................ 117
Figure 5.11: Approximate interface velocity (a), contact angle (b), forces acting on the bubble (c) and bubble dimensions (d) for a static mean contact angle of $54.5^\circ$. ................................................ 119
Figure 5.12: Approximate interface velocity (a), dynamic contact angle (b), forces acting on the bubble (c) and bubble dimensions (d) for an apparent contact angle as a function of the contact line velocity with $umax = 0.015$m/s ........................................................ 121
Figure 5.13: Approximate interface velocity (a), dynamic contact angle (b), forces acting on the bubble (c) and bubble dimensions (d) for an apparent contact angle as a function of the force balance ........................................................ 123
Figure 5.14: Contact angle vs time for $\Delta T = 7K$, from Ramanujapu and Dhir (1999) .................. 125
Figure 5.15: Bubble diameter vs time $\Delta T = 7K$, from Ramanujapu and Dhir (1999) .................. 126
Figure 5.16: Latent heat transfer for different contact angle models ........................................ 128
Figure 5.17: Conductive heat transfer for different contact angle models ........................................ 128
List of Tables

Table 2.1: Single bubble cycle .................................................................28
Table 2.2: Static contact angles $\theta_{CA}$ for distilled water at polished surfaces .........29
Table 2.3: Static contact angle $\theta_{CA}$ for distilled water at thermally or chemically treated polished surfaces .................................................................29
Table 3.1: Young-Laplace pressure drop across liquid vapor interface. ..................79
Table 4.1: Profiles of the applied interface velocity .........................................99
Table 5.1: Bubble characteristic at departure for various test cases .....................126
Chapter 1
General introduction

Boiling; a liquid vapor phase change process has been the subject of an enormous amount of studies which have lead to more empirical results than knowledge on the physical mechanisms that govern the phenomena. The field is still governed by empirical correlations that are in practice and are required for design purposes. However it is now accepted that studies focused on the physics of this very complex process will be required for further progress. This trend is on one hand supported by new experiments that take advantage of the growing capacities in data acquisition, storage and processing by computers in connection with miniaturized sensors and high speed camera and other optoelectronic facilities which are doubtless unavoidable in this field, and on the other by better and new mathematical tools which have been developed in recent years. Thus, the basic mechanisms of boiling can now be more profoundly explored leading to results that are being increasingly used to develop heat transfer models that are based on physics. As compared to the empirical correlations these models are more generally more valid. In this way we are able to create a better a chance to develop enhanced heat transfer surfaces systematically and not by trial and error methods by acquiring a deeper understanding of the governing physical mechanisms.

Most energy conversion systems and heat exchangers use boiling heat transfer, which is also employed in the thermal control of compact devices that have high heat dissipation rates. Applications of this type include the use of boiling to cool electronic components in mainframe computers and the use of compact evaporators and condensers for thermal control of aircraft avionics and spacecraft environments. The virtually isothermal heat transfer associated with boiling and condensation process makes their inclusion in power and refrigeration cycles highly advantageous from a thermodynamic efficiency viewpoint. The y are of critical importance to nuclear power plant design, both because hey are important in normal operating circumstances and because they dominate many of the accident scenarios that are studied in detail as part of design evaluation.

Liquid vapor phase change processes are also encountered in petroleum and chemical processing, liquefaction of nitrogen and other gases at cryogenic temperatures and during evaporations of precipitation of water in the earth’s atmosphere. The use of boiling heat transfer is motivated by the high efficiency of heat exchange during the nucleate boiling process. Nucleate pool boiling refers to boiling under natural convection conditions in contrast to flow boiling where liquid flow over the
surface heater is imposed by external means. Flow boiling can include external and internal flow boiling.

Nucleate pool boiling is characterised by the onset of cyclic growth and departure of vapour bubbles from a discrete site on a heated surface and is therefore greatly influenced by the bubble growth mechanism. Consequently for mechanistic modelling, it is necessary to be able to predict data for a single bubble nucleation which involves the mechanics of multiphase fluids as well as the dynamics of phase transition. The study of bubble dynamics is a coupled problem as the heat transfer determines the rate of evaporation which in turn controls the dynamics of the interface.

The nature of the interface between two fluids has been the subject many investigations. Initially the interface between two fluids was represented as a surface of zero thickness and endowed with physical properties such as surface tension. Boundary conditions on the interface were used to represent physical processes occurring at the interface, like the Young-Laplace equation relating the pressure jump across an interface to the product of surface tension and curvature of the interface.

In the case where the interface is a plane of discontinuity that separates regions of different phases, tracking it as a function of time becomes a challenging task. This is especially so, if the interface merges, disappears and/or develops holes — in other words, if it develops topological singularities. The main problematic of solving the boiling flow is thus to take into account the interface as a moving boundary. In addition the boiling process has all the complexity of single phase convective transport, i.e. nonlinearities, transition to turbulence, three-dimensional and time varying behaviour.

To overcome such problems one typically resorts to level set methods (LSM). The level set method considers an interface moving under a given velocity field (which depends on position, time, geometry of the interface, and so on). A smooth field $\Phi$ is defined and the contour where $\Phi = 0$ is defined as the interface. The evolution equation for the interface is then given by evolving $\Phi$ with the given velocity field and tracking regions of $\Phi = 0$. A complete numerical simulation of a growing and departing bubble during partial nucleate boiling was performed by Son et al. (1999) by employing the level set method (LSM), which can handle the bubble departure process.

Since then the level set method has been used by various researchers for studying boiling related phenomena. A persistent problem with the level set method is that it leaks phase, i.e. some portion of one fluid seeps into the other fluid, typically from the less dense to the denser. Particularly, when there is a steep contrast between the density and viscosity of the two interacting fluids. In the present
work a conservative level set method is formulate and employed to simulate the dynamics of a single vapour bubble at the onset of nucleate pool boiling.

1.1 Outline of the thesis

- **Chap. 2 – Literature review.**
  We present the background, context and a very brief history of the nucleate pool boiling process as well the numerical methods employed to study it. At the end we motivate the choice of the level set method for simulating single bubble dynamics.

- **Chap. 3 – Numerical modelling**
  We describe the conservative level set method, the dynamic contact angle models and the governing equations of our model. The implementation of the model is discussed and the implemented model is validated using results for known problems. The phase conservation characteristics of the model are scrutinized.

- **Chap. 4 – Decoupled bubble dynamics**
  The validated conservative level set model is applied to the study of a growing and departing vapor bubble decoupled from energy conservation equation, with phase change being simulated by direct vapor injection on the interface near the contact line. The approach is used to study the effect of local phenomena near the contact line on global dynamics of bubble.

- **Chap. 5 – Coupled bubble dynamics**
  The numerical model is used to study the growth of single bubble on a heated surface. Dynamic angle models are considered and the force-balance based dynamic contact angle is substantiated.

- **Chap 6. – Concluding Remarks**
  We finalize the thesis by summarizing the work realized during the course this study and discussing possible further development of the code as well as further application areas.
Chapter 2

Literature review

In this chapter a review of the fundamentals of boiling is presented together with the numerical methods used to predict the phenomena. Boiling is probably the most investigated phenomenon in the thermal sciences over 80 years. Experimental data have been collected, e.g. Jakob and Fritz (1931), Nukiyama (1934), Yamagata et al. (1955), Kurihara and Myers (1960), Gaertner and Westwater (1960), Siegel and Keshock (1964), Gaertner (1965), Cooper and Lloyd (1969), Nishikawa et al. (1974), Cornwell and Brown (1978), Stephan & Abdelsalam (1980), Sultan and Judd (1983), Gorenflo et al. (1986), Lienhard (1988), Wang and Dhir (1993a,b), Chen and Hsu (1995), Auracher and Marquardt (2002) and Buchholz et al. (2006) etc. We begin our review with a presentation of the different boiling heat transfer regimes with the help of the classical representation of the Nukiyama curve. Then we describe more precisely the main characteristics of the different regimes by highlighting the different physical processes occurring in a near wall region, followed by a narrative of bubble dynamics and an introduction of the numerical methods used to study it.

Driven by the necessity to understand this complex phenomenon many studies have been carried on boiling and quite a few reviews of boiling processes have appeared. For more exhaustive treatments of boiling heat transfer, the following books are recommended for consultation: Rohsenow (1973, 1985, 1998), van Stralen and Cole (1979), Carey (1992), Collier and Thome (1994), Kandlikar, Shoji and Dhir (1999) and Incropera and DeWitt (2006).

2.1 Boiling and boiling curve

When heat is applied to a surface in contact with a liquid, if the wall temperature is sufficiently above the saturation temperature, boiling occurs on the wall. Liquids having temperature larger than the saturation temperature corresponding to the local pressure are called superheated liquids. Superheated liquids are unstable and start to disintegrate. This process is in generally called flashing. The process of rupturing a continuous liquid by decrease in pressure at roughly constant liquid temperature is often called cavitation - a word proposed by Froude. The process of rupturing a continuous liquid by increase the temperature at roughly constant pressure is often called boiling. The fluctuation of molecules having energy larger than that characteristic for a stable state causes the formation of clusters of molecules, which after reaching some critical size are called nuclei. Boiling may occur
under quiescent fluid conditions, which is referred under gravity as nucleate pool boiling, or under forced-flow conditions, which is referred to as forced convective boiling.

Let us consider the heat transfer process from a heated solid to a boiling fluid. The pool boiling experimental set-up consists of a boiling fluid contained in a pool and it therefore does not include any external mean flow. The heating solid is either a plane plate, a wire, a ribbon or one of the bounding walls of the pool. It is required that its dimensions exceed the characteristic dimension of the vapor inclusion (typical bubble radius) in order to ignore size effects. In the remainder of this study, we consider by default the pool boiling of pure fluids with a heated lower horizontal wall with a mean temperature ‘T’ at the bottom of the pool that and ‘q’ being the amount of heat transmitted through the solid-fluid contact area (Figure 2.1). Note that the temperature of the boiling liquid is nearly constant except at the surface of the heated wall. At the heated surface the liquid temperature increases sharply.

Figure 2.1: Temperature distribution in pool boiling

Since we describe boiling systems as a heat exchange process, it is natural to characterize the wall temperature by $\Delta T = T_s - T_{sat}$, Where $T_s$, $T_{sat}$ and $\Delta T$ are respectively called the surface temperature, saturation temperature and wall superheat. When heating a surface in a large pool of liquid, the heat flux is usually plotted versus the wall superheat. The boiling curve was first constructed by Nukiyama (1934), he used a nichrome wire immersed in a bath of water. As he increased the power to the wire, he noticed bubbles forming at an excess temperature, $\Delta T$ of about 5°C. As he increased power further, he noticed that the power supplied to the wire could be increased greatly without a large
increase in temperature. As he increased the power further still, the temperature suddenly increased dramatically, and the wire reached its melting point. After experimenting with a platinum wire with a higher melting point, he noted that the heat flux and temperature were related, as shown in Fig 2.2.

![Figure 2.2: The Nukiyama boiling curve for saturated water. Adapted from Incropera and DeWitt (2006) using the data of Nukiyama (1934)](image)

Nukiyama believed that a method of temperature control of ΔT, instead of a power-controlled method, would yield a better curve. Drew and Mueller (1937) performed the experiment using a steam pipe and obtained a curve similar to that shown in Figure 2.3. This figure shows the relationship of heat flux and temperature for most liquids. A typical Nukiyama curve has four distinct heat transfer regimes between which are three transition points.

The four distinct heat transfer regimes are natural convection and nucleate, film and transition boiling regimes. The three transition points are the onset of nucleate boiling (ONB), departure from nucleate boiling (DNB) and the beginning of the film boiling regime at the point of minimal heat flux (MHF). These are shown in the following figure.
2.1.1 Natural convection regime

Fluid surrounding the heated solid receives heat, becomes less dense and rises due to buoyancy. The surrounding, cooler fluid then moves in to replace it, which is then heated and the process continues, forming a convection current. This process transfers heat energy from the bottom of the pool to top. The process is characterized by single-phase natural convection from the hot surface to the saturation liquid without formation of bubbles on the surface. Bubbles do not form in this region because there is not enough vapor in contact with the liquid. Natural convection terminates at the first transition point called incipience of boiling or onset of nucleate boiling (ONB), at which the first individual bubbles appear on the heated surface leading to the nucleate boiling regime.
2.1.2 Nucleate boiling regime

The nucleate boiling regime corresponds to low wall superheats $T$ and to a limited range of wall heat flux $q$. The lower limit in terms of both $q$ and $\Delta T$ is the onset of nucleate boiling (ONB) and thus corresponds to the upper limit of the convective regime\(^1\). ONB corresponds to a transition between the non-boiling and the boiling regimes.

\(^1\) We underline that the heat exchange corresponds to the phase change and convective energy contribution.
The formation of the vapor bubbles in the NB regime is the result of successive nucleation events and consecutive heterogeneous bubble growth dynamics until the departure of the bubble from the wall. The major part of the wall is in contact with the liquid phase even if high void fractions can be reached right above the wall. As a consequence, the wall superheat is low (since liquid temperature cannot reach large superheats values). Due to the agitation associated with bubble growth and motion, the efficiency of the convective heat exchange is greatly enhanced with regard to a single-phase case.

During natural convection, the wall temperature rises as the heat flux is increased until the first bubbles form (or nucleate) at small cavities in the heated surface, called nucleation sites, leading to nucleate boiling regime. By increasing the heat flux, more nucleation sites become activated. Thus at low heat fluxes the surface is covered with bubbles that grow and depart in quick succession (figure 2.4).

By increasing the heat flux even further, the rate of departing bubbles becomes more rapid until the bubbles appear to coalesce into vapor jets, (figure 2.5) that is, bubbles form, separate, and reform so quickly that continuous streams or vapor columns are seen. The heat flux increases dramatically for relatively modest increases in $\Delta T_{\text{sat}}$, changing the slope of the nucleate boiling curve.
A further increase in $q$ eventually prohibits the liquid from reaching the heated surface, which such that blanketing of the heated surface by vapor occurs (figure 1.6), accompanied by a rapid rise in the surface temperature to dissipate the applied heat flux. This limit of the NB regime associated with high values of $q$ is called departure from nucleate boiling (DNB) and corresponds to a transition between the different boiling regimes. The associated value for the heat flux is called the critical heat flux (CHF).

Following DNB, the process follows a path that depends on the manner in which the heat flux is applied to the surface.
For heaters that impose a heat flux at the surface, such as electrical-resistance elements or nuclear fuel rods, the process progresses on a horizontal line of constant heat flux so that the wall superheat jumps to the corresponding point on the film boiling part of the curve.

When the wall temperature is the externally controlled variable, such as by varying the saturation temperature of steam condensing inside a tube with boiling on the outside, the process path moves from the DNB to the minimal heat flux (MHF) point, and vice versa, following the transition boiling path.

### 2.1.3 Film boiling regime (FB)

If at departure from nucleate boiling, the heat flux is increased above the CHF value, the system shifts to the film boiling regime (FB). The FB regime corresponds to very high values of the wall superheat and to heat transfer coefficients that are lower than in the NB regime. The transition from NB to FB is characterized by a very sudden and very large increase of the wall temperature. Typically the order of magnitude of this increase can reach several hundreds of Kelvin. An ulterior increase in heat flux $q$ may bring the surface to the burnout point (BO), where the surface temperature reaches the melting point of the heater. This phenomenon is also termed as the boiling crisis.

In the FB regime, the surface becomes dry and the wall is covered by a vapor film. The vapor bubbles no longer grow and depart from the heater surface but from the vapor–liquid interface of the vapor layer. At the liquid-vapor interface, a dynamic process of vapor generation and release occurs. Due to the Rayleigh Taylor instability (RTI), the surface of the vapor film is wavy and is the location of a cyclic process of bubble formation as represented on figure 1.7.

The vapor film is stable in the sense that liquid does not normally wet the heater surface and relatively large bubbles are formed by evaporation at the free vapor–liquid interface, which then depart and rise up through the liquid pool. The heat flux is transmitted from the wall to the liquid-vapor interface (whose temperature can be approximated by the saturation temperature) through a combination of radiative, conductive and convective transfers across the vapor layer. Conduction takes place across the vapor film while radiation occurs from the wall to the liquid or to the walls of the vessel.
Figure 2.9: Film boiling regime (FB)

The low value of the vapor thermal diffusivity (with regard to the liquid one), explains the higher wall temperature in the FB regime than in the NB regime. The order of magnitude of the very large and very sudden increase of the wall temperature, that characterizes the transition from NB to FB, can typically reach several hundreds of Kelvin. An ulterior increase in heat flux $q$ may bring the surface to the burnout point (BO), where the surface temperature reaches the melting point of the heater. This phenomenon is also termed as the boiling crisis.

If we reduce the heat flux after arriving at FB from NB at CHF, then the film boiling curve passes below the CHF line until reaching the MHF point. Here again, the process path depends on the mode of heating. For an imposed heat flux, the process path jumps horizontally at constant $q$ to the nucleate boiling curve NB. Consequently, a hysteresis loop is formed when heating a surface up past the DNB and then bringing it below MHF when $q$ is the boundary condition imposed.

### 2.1.4 Transition boiling regime (TB)

The lower limit of FB is characterized by the minimal heat flux (MHF) that corresponds to the transition to the third boiling regime, the transition boiling (TB). The domain of existence of TB joins the CHF and the MHF points and concerns intermediate values of wall temperature. For this regime, the local wall heat flux and/or temperature fluctuate violently around their mean values. For these reasons, TB is hard to characterize in itself and is often modeled as an unstable mix between the NB and FB regimes. Thus, in transition boiling the process is considered to vacillate between nucleate boiling and film boiling, where each mode may coexist next to one another on the heated surface or may alternate at the same location on the surface. It is worth noting that steady-state TB regime can
be experimentally reached by imposing the wall temperature and not the heat flux. If the heat flux \( q \) is experimentally imposed, this regime is unstable and therefore inaccessible.

At the MHF, while decreasing \( \Delta T \) and coming from the TB regime, the film configuration becomes unstable and locally breaks (i.e. locally some liquid comes into contact with the wall). As a consequence, wetted (covered by the liquid phase) area appears on the solid surface. In the transition boiling regime, the fluid/solid contact surface is the place of large and intermittent wetting and drying dynamics, i.e. it is covered alternatively by the liquid (wet) or the vapor (dry) phases. These hydrodynamic events are related to the large fluctuations of \( \Delta T \) and \( q \).

![Figure 2.10: Transition Boiling Regime](image)

### 2.2 Length scales

In order to study the physical mechanisms associated with nucleate pool boiling, we first introduce three different length scales as determining three levels of description of the nucleate boiling process. Each of this levels being related to a different typical length scale for the bubble description. For each scale different physical mechanisms can be identified.

In the previous section, we have distinguished the different regimes of the pool boiling by considering the process in a near wall region. The typical size of this region is of the order of magnitude of a few bubble diameters. This sets the bubble as the natural basic element of the nucleate boiling process. The three different length scales can be defined from three different levels of modelling bubbles. At the first level of description, denoted as ‘two phase flow scale’, the bubbles are considered as fixed in geometry and size. This is mainly relevant far from the wall, i.e. when the main part of the bubble growth is achieved. This level of description therefore ignores the bubble growth dynamics. At the
second level of description, denoted ‘mean bubble growth scale’, the bubbles are considered as fixed in geometry but not in size. For instance the bubble is assimilated to a sphere whose size depends on time, the dynamics of bubble formation is therefore taken into account. At the third level of description, denoted ‘local scale’, both the geometry and the size of the bubble are considered as time dependent. The dynamics of bubble formation area therefore described more precisely (with more degrees of freedom) than at the ‘mean bubble growth scale’. An illustration of these three levels of description of the nucleate boiling process is provided in figure 2.9.

Figure 2.11: The length scales of description of nucleate boiling, (a) Two phase flow scale (b) Mean bubble growth scale and (c) Local scale

2.2.1 Two phase flow scale

In our classification this scale is the largest one and is associated with the most idealized level of the modeling of the nucleate boiling process. The basic picture considers a population of bubbles coming from the wall and having constant size and geometry. Mean space and time frequencies of bubble emission are modeled. The rate of vapor incoming from the wall is related to the value of the wall heat flux q. It is worth noting that this scale does not actually ‘see’ the wall. This kind of large scale analysis of the boiling flows has been used for example by Zuber (1963) to derive a correlation for the low heat transfer nucleate boiling regime (region of isolated bubbles, where bubbles do not interact with each other). At larger heat flux, bubbles become so numerous that their interactions are no longer negligible. The large number of individual bubbles generated in the near wall region coalesce each other and somewhat form big masses of vapor flowing away from the wall. These big masses can be idealized by a somewhat continuous vapor channel, the vapor columns. The model of the two-
phase flow far above the wall is therefore idealized by a counter-current flow of vapor inside these
channels and of liquid around those columns. The reader interested by this approach can refer to

2.2.2 Mean bubble growth scale
At this scale, the near wall nucleate boiling process is described in a way that facilitates the
evaluation of bubble formation through modelling. The characteristic scale of this level of description
is that of the bubble, which is regarded as having a fixed geometry but varying in size allowing us to
model it growing on the wall. From the study of the bubble growth process, several heat-exchange
mechanisms can be identified including the transport of latent heat thus permitting us to model more
accurately the various phenomena involved in the fluid wall heat exchange. The influence of physical
phenomena occurring in a near wall region (that were ignored at the two-phase flow scale) are
therefore entering the model.

At this level of description the nucleate boiling process is idealized as a set of sub-phenomena. The
main one is the cyclic process of bubble formation near the heated wall. It is idealized by a sequence
of events (nucleation, growth, departure). Each of these sub-phenomena has been the object of
specific studies, either based on analytical models or on correlation issued from experimental
observations. The creation of bubbles is modelled as a cyclic process localized on sites and consisting
of the following events: nucleation, growth, departure, and waiting. Some models also consider the
interaction between sites. This scale of analysis covers a wide range of phenomena listed below:

1. partition of the wall heat flux between different heat transfer processes
   (a) latent heat transport (evaporation) (eventually two parts around bubble and
       micro-layer contribution)
   (b) transient conduction
   (c) natural convection
2. spatial frequency of the bubble formation process, the nucleation site density
3. bubble growth rate
4. bubble departure size
5. waiting time
6. bubble interactions: thermal, hydrodynamic, and coalescence

2.2.3 Local scale

The mean bubble growth scale describes the mean bubble formation process in an idealized way which is relevant at low heat flux NB regime. However at high heat flux bubbles are more spread over the wall before their departure. This bubble behavior is very different from the regular behavior. The model of nucleate boiling process at the mean bubble scale is too rigid to describe such a behavior (according to the fact that the bubble shape is imposed to be either spherical or hemispherical). We must therefore consider a smaller level of modeling of the NB process. The present level of description takes into account the full time and space dependency of the bubble shape. It is worth noting that the amount of modeling is therefore quasi-vanishing since we now consider the full set of non-isothermal Navier-Stokes equations and interface jump conditions. The main physical mechanisms that are taken into account at the local scale in addition to the physical mechanisms considered at the mean bubble growth scale are listed below.

1. Local curvature of the bubble and capillary forces
2. Pressure recoil at the interface: the jump in pressure \( p = -\dot{m}/\rho \), where \( \dot{m} \) is the local mass transfer rate.
3. Triple line dynamics (static-dynamic contact angle) and associated quasi-singular heat transfer (cf. Anderson and Davis (1994) or Mathieu et al. (2004)
4. Gravity: effect of the hydrostatic pressure gradient on the bubble shape and consequently on its departure dynamics (cf. Shikhmurzaev (1999) whose model considers the time dependent shape of the bubble and also includes a model for the contact line dynamics)
5. Local heat conduction problem inside the area of contact between wall and vapor at the dry base of a bubble (cf. Blum et al. (1999))

To take into account the whole set of mechanisms and the complex time dependent geometry of the bubble at this level of description, it is required to use numerical methods. Several numerical simulations of bubble growth dynamics using different numerical methods can be found in the literature, e.g. Son et al. (1999, 2002) for the level-set method, Welch and Wilson (2000) for the VoF method, Juric and Tryggvason (1998) for the front tracking method. While Yang et al. (2001) used a
Lattice-Boltzmann model based numerical method for simulating film boiling regime where as Fouillet and Jamet (2005) sued a diffuse interface method approach for the same regime.

As a partial conclusion, in order to describe certain features of the nucleate boiling regime at high heat fluxes, it is necessary to consider the full problem of the bubble growth as having a time dependent geometry.

### 2.3 Bubble dynamics

A thorough understanding of the process of boiling heat transfer in pool boiling requires an investigation of the thermodynamics of bubbles and the hydrodynamics of the flow resulting from the departure of the bubbles from the heater surface. The growth of vapor bubbles can be a particularly complex physical phenomenon. For example, bubble growth and departure are influenced by the orientation of the surface, the contact angle, the thickness and temperature profile in the thermal boundary layer, the proximity of neighboring bubbles, transient thermal diffusion within the wall to the adjacent liquid, wake effects of the previous bubble, bubble shape during growth, and so on. A vapor bubble forms and grows in a liquid as long as the bubble vapor pressure is higher than the ambient liquid pressure, that is, \( p_v > p_l \). Stability is reached when \( p_v - p_l = \frac{2\sigma}{r} \) which forms a bubble in equilibrium and is known as the Youngs-Laplace law.

Boiling is a cyclic process. The life of a single bubble is summarized in Table 2.1. The ebullition cycle described in the table is followed by a waiting period, which occurs at the nucleation site just after the departure of a bubble and before a new bubble is formed. This was showed by a shadowgraph and Schlieren technique (Hsu and Graham, 1961). They produced an explanation for the ‘waiting time’ of bubbles formed on a heated surface by boiling. The bubble departure ruptured the thermal boundary layer, and a new bubble was formed only after the effects of the disturbance had disappeared. Hsu (1962) developed a model based around the so-called ‘waiting time’ required for the liquid to attain the necessary superheat. The nucleation proceeds when the thermal boundary layer thickness reaches a critical fraction of the nucleus radius. This waiting period between two consecutive bubbles can be described meaningfully only in the lower heat flux range where the bubbles are discrete. A comprehensive treatment of bubble growth theory can be found in the book by van Stralen and Cole (1979).
Nucleation is a molecular scale process in which a small bubble (nucleus) of a size just in excess of the thermodynamic equilibrium is formed.

Initial growth from the nucleation size is controlled by inertia and surface tension effects. The growth rate is small at first but increases with bubble size as the surface tension becomes less significant.

Heat transfer becomes increasingly important while inertia effects lose significance until bubble reaches an asymptotic growth stage where it is controlled by the rate of heat transferred from the surrounding liquid to facilitate the evaporation at the bubble interface.

If the bubble during its growth encounters subcooled liquid, it may collapse. The controlling phenomena for the collapse are much the same as for the growth but are encountered in the reverse order. Otherwise the bubble departs from the heater surface.

### Table 2.1: Single bubble cycle

Bubble dynamics play a key role in the development of any analytical model purporting to predict nucleate pool boiling heat transfer coefficients. The simplest case to analyze is that of a single spherical bubble growing within an infinite, uniformly superheated liquid remote from a wall. Before we describe the cycle of single bubble it is important to highlight the role of the contact angle.

### 2.3.1 Contact angle

The contact angle characterizes the molecular interaction between the liquid and the solid surface. It is the angle between the tangent to the interface and the wall. Hydrophobic surfaces, $\theta_{CA} > 0$, cause heterogeneous nucleation at much reduced pressure difference. In the study of bubble dynamics two types of contact angles are considered, static and dynamic.

**Static contact angle:** The shape of a bubble in a static state or a state of equilibrium on a heated surface depends on the material properties of the liquid surrounding the bubble, the vapor inside it and the surface on which it is resting. This dependency is usually described as a function of the
interfacial tensions using the equation first derived by Thomas Young (1805). Young’s equation
governs the equilibrium of the three interfacial tensions and the Young contact angle, \( \theta_{CA,Y} \):

\[
\theta_{CA,Y} = \cos^{-1}\left(\frac{\sigma_{sv} - \sigma_{sl}}{\sigma_{lv}}\right)
\]  

(2.1)

Where \( \sigma \) is the surface tension between solid-vapor (sv), solid-liquid (sl) and liquid-vapor (lv) surfaces. The following tables give some information on how the contact angle can change for
different wall materials and different surface preparation procedures.

<table>
<thead>
<tr>
<th>Material</th>
<th>( \pi / )</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steel</td>
<td>3.7</td>
<td>Siegel and Keshock (1964)</td>
</tr>
<tr>
<td>Nickel</td>
<td>4.74 to 3.83</td>
<td>Siegel and Keshock (1964)</td>
</tr>
<tr>
<td>Chrome-Nickel Steel</td>
<td>3.7</td>
<td>Arefeva and Aladev (1958)</td>
</tr>
<tr>
<td>Zinc</td>
<td>3.4</td>
<td>Arefeva and Aladev (1958)</td>
</tr>
<tr>
<td>Bronze</td>
<td>3.2</td>
<td>Arefeva and Aladev (1958)</td>
</tr>
<tr>
<td>Copper</td>
<td>4</td>
<td>Arefeva and Aladev (1958)</td>
</tr>
<tr>
<td>Copper</td>
<td>3</td>
<td>Gaertner and Westwater (1960)</td>
</tr>
<tr>
<td>Copper</td>
<td>2</td>
<td>Wang and Dhir (1993b)</td>
</tr>
<tr>
<td>Stainless steel 304 (25°C)</td>
<td>2.25</td>
<td>Hirose et al. (2006)</td>
</tr>
<tr>
<td>Zircaloy (25°C)</td>
<td>2.46</td>
<td>Hirose et al. (2006)</td>
</tr>
<tr>
<td>Aluminum (25°C)</td>
<td>2</td>
<td>Hirose et al. (2006)</td>
</tr>
</tbody>
</table>

Table 2.2: Static contact angles \( \theta_{CA} \) for distilled water at polished surfaces.

<table>
<thead>
<tr>
<th>Material</th>
<th>( \pi / )</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Copper heated to 525 K and exposed to air one hour:</td>
<td>5.14</td>
<td>Wang and Dhir (1993b)</td>
</tr>
<tr>
<td>Copper heated to 525 K and exposed to air two hour:</td>
<td>10</td>
<td>Wang and Dhir (1993b)</td>
</tr>
<tr>
<td>Chrome-Nickel Steel chemically treated:</td>
<td>2.9</td>
<td>Arefeva and Aladev (1958)</td>
</tr>
</tbody>
</table>

Table 2.3: Static contact angle \( \theta_{CA} \) for distilled water at thermally or chemically treated polished surfaces.
**Dynamic contact angle:** In nucleate pool boiling bubbles nucleate at the heated surface and stay attached to it through out their growth period. Smoothness; homogeneity and rigidity of the solid surface are underlying assumptions of the Young’s equation which also implies that that the solid should be chemically and physically inert with respect to the liquids to be employed. Thus a unique contact angle is expected for a given system.

However, it has been experimentally observed that the contact angle made by the liquid–vapor interface at the bubble base with the wall varies during bubble growth and departure stages. Thus in a real system a spectrum of contact angles ranging from the advancing contact angle, $\theta_{ACA}$, to the receding contact angle, $\theta_{RCA}$, are detected. The upper limit of the spectrum is the advancing contact angle, $\theta_{ACA}$, which is the contact angle found at the advancing edge of the liquid. The lower limit is the receding contact angle, $\theta_{RCA}$, which is the contact angle found at the receding edge. The difference between the advancing and receding contact angles is known as the contact angle hysteresis, $\theta_{hyst}$:

$$\theta_{hyst} = \theta_{ACA} - \theta_{RCA} \quad (2.2)$$

The variation of the contact angle may influence the characteristics of bubble dynamics and is therefore an important parameter in surface science. In consequence, for the numerical simulation of bubble dynamics, an appropriate contact angle model is essential for a correct prediction of the bubble formation.

### 2.3.2 Nucleation

The process of rupturing a continuous liquid by increasing the temperature at roughly constant pressure is often called boiling. The fluctuation of molecules having energy larger than that characteristic for a stable state causes the formation of clusters of molecules, which after reaching some critical size are called nuclei. The theory of nucleation provides us with information about the generation of nuclei per unit time and unit volume of the liquid as a function of the local parameter. It has been well established that vaporization usually begins with an embryo in the superheated liquid, Carey (1992). Once the embryo is larger than a critical size, a vapor bubble will form. The critical radius, $r_{B,c}$ can be estimated by computing the incipient nucleation temperature in pool boiling from the classical kinetics of nucleation, Cole (1974) as follows:

Homogeneous nucleation: If the vapor embryo completely forms within a superheated liquid, it is called “homogeneous nucleation”. It is usually associated with high degrees of superheat and
extremely rapid rates of vapor generation. For homogeneous nucleation in superheated liquids, the bubble nucleation density $J$ is given by:

$$J = N_0 \left( \frac{kT_n}{h} \right) \exp \left[ -\frac{16\pi\sigma}{3kT_n(p_v - p_l)^2} \right]$$  \hspace{1cm} (2.3)$$

where $T_n$, $\sigma$, $k$ and $h$ are the nucleation temperature, the surface tension, the Boltzmann constant, and the Planck constant, respectively.

Heterogeneous nucleation: On the other hand, if the vapor embryo forms at the interface between liquid and solid or gas, it is called “heterogeneous nucleation”. It can occur at lower degrees of superheat. For heterogeneous nucleation on a smooth surface with no cavity, the bubble nucleation density is:

$$J = N_0^{2/3} \psi \left( \frac{kT_n}{h} \right) \exp \left[ -\frac{16\pi\sigma^3 \omega}{3kT_n(p_v - p_l)^2} \right]$$  \hspace{1cm} (2.4)$$

with,

$$\psi = \frac{1 + \cos \theta_{CA}}{2} \hspace{0.5cm} \text{and} \hspace{0.5cm} \omega = \frac{(1 + \cos \theta_{CA})^2 (2 - \cos \theta_{CA})}{4}$$  \hspace{1cm} (2.5)$$

Where $\theta_{CA}$ is the contact angle. With the aid of Clausius-Clapeyron equation, Eqs 2.1 and 2.2 can be expressed in the following compact form, Li and Cheng (2004);

$$T_n - T_s = \left( \frac{T_s}{h/\rho_v} \right) \left( \frac{16\pi\sigma^3 \omega}{3kT_n \ln \left( \frac{N_0^{2/3}kT_n\psi}{Jh} \right)} \right)^{1/2}$$  \hspace{1cm} (2.6)$$

which is applicable for both homogeneous nucleation (with $\gamma = \psi = \omega = 1$) and heterogeneous nucleation (with $\gamma = 2/3$ and $\psi$ and $\omega$ given by Eq 2.3). The nucleation temperatures for homogeneous and heterogeneous nucleation can be obtained from Eq. (2.4) iteratively if the value of $J$ is known. Note that the nucleation temperature determined from Eq. (2.4) is not sensitive with the chosen value of $J$. After the nucleation temperature is obtained, the critical bubble radius for homogeneous and heterogeneous nucleation is given by;
\[ r_{B,c} = \frac{2\sigma}{p_{\text{sat}}(T_\text{n}) - p_l} \]  

(2.7)

For water at the atmospheric pressure, the homogeneous nucleation temperature and the critical bubble radius determined from Eqs. (2.4) and (2.5) are: \( T_n = 303.71^\circ\text{C} = 576.8\text{K} \) and \( r_{B,c} = 3.15 \text{nm} \).

### 2.3.3 Bubble growth

A spherical bubble growing in a uniformly superheated liquid is the simplest geometry to analyze. The pressure and temperature of the vapour region inside the bubble are \( p_V \) and \( T_V \); the bubble radius is \( r_B \) and is a function of time \( t \) from the initiation of growth (growth rate is \( \frac{dr_B}{dt} \)). The pressure and temperature in the liquid are \( p_l \) and \( T_l \). In this analytical model other effects influencing the bubble are ignored, such as the static head of the liquid, and the center point of the bubble is assumed to be immobile.

At inception, the superheat is sufficient for nucleation. Then, as the bubble grows, the pressure inside the bubble decreases and with it, \( T_{\text{sat}} \) at the bubble interface. Enthalpy stored in the superheated liquid adjacent to the interface is converted into latent heat at the bubble interface and hence the interfacial temperature falls, creating a thermal diffusion shell around the bubble. Momentum is imparted to the surrounding liquid as the bubble grows and heat diffuses from the superheated bulk to the interface at a rate equal to the rate at which latent heat is liberated at the interface.

In addition, the equilibrium vapor pressure curve is assumed to describe this dynamic process, and it is assumed that the vapor pressure in the bubble corresponds to the saturation pressure at the vapor temperature [i.e., that \( p_V = p_{\text{sat}}(T_V) \)]. Bubble growth under these conditions is controlled by two factors:

1. **Inertia.** The initial growth of a bubble is very fast, limited only by the momentum available to displace the surrounding liquid from its path. That is, inertia must be imparted to the liquid to accelerate it away in front of the growing bubble.

2. **Heat diffusion.** As the bubble grows in size, the effect of inertia becomes negligible, and growth continues by virtue of diffusion of heat from the superheated liquid to the interface, although at a much slower growth rate than during the inertia-controlled stage of growth.
For inertia-controlled bubble growth during the initial stage of bubble growth, Rayleigh (1917) modeled incompressible radially symmetric flow of the liquid surrounding a bubble for a spherical bubble with a differential element of radius \( r \) and thickness \( dr \) for a bubble of radius \( r_b \). The Rayleigh equation is:

\[
\frac{d^2 r_b}{dt^2} + \frac{3}{2} \left( \frac{dr_b}{dt} \right)^2 = \frac{1}{\rho_L} \left( p_V - p_L - \frac{2\sigma}{r_b} \right)
\]  
(2.8)

Where the vapor pressure in the bubble is \( p_V \) and that at the interface is \( p_L \). Since \( 2\sigma/r_b \ll p_V - p_L \), the term \( 2\sigma/r_b \) can be ignored. Using a linearized version of the Clapeyron equation for the small pressure differences involved, the Rayleigh equation reduces to:

\[
\frac{d^2 r_b}{dt^2} + \frac{3}{2} \left( \frac{dr_b}{dt} \right)^2 = \frac{\rho_V}{\rho_L} \left( \frac{T_L - T_{sat}(p_L)}{T_{sat}(p_L)} \right) h_{LV}
\]  
(2.9)

Integrating from the initial condition of \( r_b = 0 \) at \( t = 0 \), the Rayleigh bubble growth equation for inertia-controlled growth is obtained:

\[
r_b(t) = \left[ \frac{2}{3} \left( \frac{T_L - T_{sat}(p_L)}{T_{sat}(p_L)} \right) h_{LV} \frac{\rho_V}{\rho_L} \right]^{1/2} \quad t
\]  
(2.10)

For heat diffusion–controlled growth, Plesset and Zwick (1954) derived the following bubble growth equation for relatively large superheats:

\[
r_b(t) = J_0 \left( \frac{12a_L t}{\pi} \right)^{1/2}
\]  
(2.11)

Where \( a_L \) is the thermal diffusivity of the liquid:

\[
a_L = \frac{\lambda_L}{\rho_L c_{pl}}
\]  
(2.12)

and the Jakob number is;
Thus, for heat diffusion–controlled bubble growth, the radius $R$ increases with time as $t^{1/2}$, while it grows linearly with time during the initial inertia-controlled stage of growth. Mikic et al. (1970) combined the Rayleigh and Plesset–Zwick equations to arrive at an asymptotic bubble growth equation valid for the entire bubble growth period:

$$r_B^+ = 2 \left[ \left( t^+ + 1 \right)^{3/2} - \left( t^+ \right)^{3/2} - 1 \right]$$  \hspace{1cm} (2.14)

Where,

$$r_B^+ = \frac{r_B^A}{B^2}$$  \hspace{1cm} (2.15)

$$t^+ = \frac{tA^2}{B^2}$$  \hspace{1cm} (2.16)

$$A = \left[ \frac{2}{3} \left( \frac{T_L - T_{sat}(p_L)}{T_{sat}(p_L)} \right) h_{LV} \frac{\rho_v}{\rho_L} \right]^{1/2}$$  \hspace{1cm} (2.17)

$$B = \left( \frac{12a_L}{\pi} \right)^{1/2} Ja$$  \hspace{1cm} (2.18)

The expression (2.14) reduces to equations (2.10) and (2.11) at the two extremes of $t^+$.

Bubble growth at heated walls differs significantly from these ideal conditions since growth occurs in a thermal boundary layer that may be thicker or thinner than the bubble itself.
The velocity field in the liquid created by the growing bubble is affected by the wall and with it the inertia force imposed on the liquid, which may change the bubble shape from spherical to hemispherical or to some other more complex shape. The hydrodynamic wake of a departing bubble may disturb the velocity field of the next bubble or that of adjacent bubbles. Furthermore, rapidly growing bubbles trap a thin evaporating liquid microlayer on the heated surface. For example, Fig. 2.12 illustrates microlayer evaporation underneath a growing bubble and macrolayer evaporation from the thermal boundary layer to the bubble as proposed in a model by van Stralen (1966).

### 2.3.4 Bubble departure

Bubble departure is another fundamental process of importance in nucleate boiling. The tangential shear due to the volume- and time-averaged pulsation velocity caused by the thermally controlled bubble growth is found to be responsible for the natural switch from isolated bubble growth into departure as the temperature difference between the bubble interface and the surrounding liquid increases.

The diameter at which a bubble departs from the surface during its growth is controlled by buoyancy and inertia forces (each attempting to detach the bubble from the surface) and surface tension and hydrodynamic drag forces (both resisting its departure). Furthermore, the shape of the bubble may deviate significantly from the idealized spherical shape. While slowly growing bubbles tend to remain spherical, rapidly growing bubbles tend to be hemispherical. Numerous other shapes are observed using high-speed movie cameras or videos.
The simplest case to analyze is that of a large, slowly growing bubble on a flat surface facing upward, for which the hydrodynamic and inertia forces are negligible. Departure occurs when the buoyancy force trying to lift the bubble off overcomes the surface tension force trying to hold it on. The surface tension force also depends on the contact angle $\alpha$ (i.e., a contact angle approaching $90^\circ$ increases the surface tension force and hence the bubble departure diameter). Fritz (1935) proposed the first bubble departure equation that equated these two forces. The Fritz equation, using the contact angle $\theta_{CA}$ (i.e., $\theta_{CA} = \pi/2 = 90^\circ$ for a right angle) and surface tension $\sigma$, gives the bubble departure diameter as:

$$D_{B,d} = 0.0208\theta_{CA}\left[\frac{\sigma}{g(\rho_l - \rho_v)}\right]^{1/2}$$

(2.19)

By considering the various forces influencing bubble growth expressions for bubble departure diameter have been developed both empirically and analytically and can be found in literature. Though, these expressions are not always consistent with each other. The role of surface tension in the determination of bubble departure diameters has been the source of some disagreement between various investigators. Generally, surface tension inhibits bubble departure by tending to push the bubble against the wall. However, Cooper et al. (1978) argued that by making the bubble spherical surface tension assisted bubble departure in some cases. Furthermore Cole & Rohsenow (1969) correlated the bubble departure diameter with fluid properties and found it to be independent of the wall superheat while the expression for bubble departure diameter proposed by Gorenflo et al. (1986) indicates weak dependency of the bubble diameter on wall superheat.

Issues regarding the forces that act on a growing bubble can be put to rest only by properly accounting for the adhesion forces and interfacial tension during complete numerical simulation of both bubble growth and departure, Dhir (1998).

### 2.3.5 Bubble release frequency

Using the bubble waiting time $t_w$ and the growth time $t_g$ expressions a theoretical evaluation of the bubble release frequency $f$ can be approximated, i.e. $f = 1/(t_w + t_g)$. As previously explained in the beginning of section 2.3 the waiting time corresponds to the time it takes for the thermal layer to redevelop so that it can allow nucleation of a bubble. However because many simplifications are made in obtaining $t_w$ and $t_g$ the predictions of bubble release frequency based on waiting and growth times do not match well with the available data, Dhir (1998). Thus both the bubble departure diameter
and the bubble release frequency are included in correlations that reported in the literature. One of the most comprehensive correlations of this type is given by Malenkov (1971).

More complex bubble departure models include the inertia, buoyancy, drag, and surface tension forces. The surface tension may also act to pinch off the bubble as it begins to depart from the surface. Keshock and Siegel (1964) assumed the following force balance of the static and dynamic forces acting on a departing spherical bubble;

\[ F_b + F_p = F_i + F_a + F_D \]  \hspace{0.5cm} (2.20)

where \( F_b \) and \( F_p \) are the buoyancy and the excess pressure forces, respectively, acting to lift the bubble off the surface and \( F_i, F_a \) and \( F_D \) are the inertia, surface tension, and liquid drag forces resisting bubble departure. The buoyancy force is;

\[ F_b = \frac{\pi D_{B,b}^3}{6} g (\rho_L - \rho_v) \]  \hspace{0.5cm} (2.21)

The excess pressure on the dry area where the bubble is attached to the wall is;

\[ \Delta p = \frac{2\sigma \sin \theta_{CA}}{D_{B,b}} + \frac{\sigma}{r_{B,b}} \]

\[ \Delta p \equiv \frac{2\pi \sigma \sin \theta_{CA}}{D_{B,b}} \]  \hspace{0.5cm} (2.22)

The first term comes from the Young-Laplace equation law applied to the bubble base diameter, including the contact angle \( \alpha \), while the second term accounts for the effect of curvature at the base of the bubble. Keshock and Siegel assumed that the second term is negligible compared to the first, such that the excess pressure force acting on the base area of diameter \( D_{B,b} \) is;

\[ F_p = \frac{\pi D_{B,b}^2 \sigma \sin \theta_{CA}}{2} \]  \hspace{0.5cm} (2.23)

The inertia force imparted on the surrounding liquid by the growing bubble is;
2.4 Heat transfer mechanisms

In this section the heat transfer mechanisms playing a role in nucleate pool boiling are described. In partial nucleate boiling, or in the isolated bubble regime, transient conduction into liquid adjacent to the wall is an important mechanism for heat transfer from an upward-facing horizontal surface (Forster & Greif 1959). These mechanisms are described below;

2.4.1 Bubble agitation

After bubble inception, the superheated liquid layer is pushed outward and mixes with the bulk liquid. The bubble acts like a pump in removing hot liquid from the surface and replacing it with cold liquid. The systematic pumping motion of the growing and departing bubbles agitates the liquid, pushing it back and forth across the heater surface, which in effect transforms the otherwise natural convection process into a localized forced convection process. Sensible heat is transported away in the form of superheated liquid and depends on the intensity of the boiling process.

![Bubble agitation](image.png)

Figure 2.13: Bubble agitation

2.4.2 Vapor-liquid exchange

The wakes of departing bubbles remove the thermal boundary layer from the heated surface, and this creates a cyclic thermal boundary layer stripping process. Sensible heat is transported away in the form of superheated liquid, whose rate of removal is proportional to the thickness of the layer, its mean temperature, the area of the boundary layer removed by a departing bubble, the bubble departure frequency, and the density of active boiling sites.
Buchholz (2005) found faster liquid temperature fluctuations with smaller amplitudes at a lower liquid temperature level for higher heat fluxes to the heater. In their study the liquid above the heater was significantly superheated with pronounced but slow temperature fluctuations at low heat flux. Thus, at low heat fluxes with a small number of active nucleation sites a significant portion of the total heat flux is transferred by convection.

### 2.4.3 Evaporation

Heat is conducted into the thermal boundary layer and then to the bubble interface, where it is converted to latent heat. Macro-evaporation occurs over the top of the bubble while micro-evaporation occurs underneath the bubble across the thin liquid layer trapped between the bubble and the surface, the latter often referred to as microlayer evaporation.

A hypothesis for the mechanism of nucleate boiling considering the vaporization of a microlayer of water beneath the bubble was first suggested by Moore and Mesler (1961). They measured the surface temperature during nucleate boiling of water at atmospheric pressure and found that the wall temperature occasionally drops 11-17°C in about 2msec. From these oscillations in the temperature measured at the bubble release site they deduced the existence of a microlayer under the bubble. This hypothesis was further verified by Sharp (1964).
The existence of a microlayer underneath isolated bubbles formed on glass or ceramic surfaces was not only confirmed by Cooper and Lloyd (1969) but its thickness was also deduced by the authors from the observed response of the heater surface thermocouple. They expressed the local thickness of the microlayer in the following form:

\[ \delta_m = \sqrt{\nu_l t} \]  

(2.24)

Where \( \nu_l \) is the kinematic viscosity of the liquid, and \( t \) is the bubble growth time. It was further demonstrated that bubble growth was mostly due to evaporation from the microlayer.

However, even after more than three decades of research, we still do not have an effective, consistent model for bubble growth on a heated surface that appropriately includes the microlayer contribution and time-varying temperature and flow field around the bubble, Dhir (1998). Plesset and Prosperetti (1976) concluded that in subcooled boiling, evaporation at the microlayer accounts for only 20% of the total heat flux. Lee & Nydahl (1989) calculated the growth of spherical bubbles with a microlayer using Cooper and Lloyd’s formulation and came to the same conclusion as Cooper and Lloyd, that microlayer evaporation is a significant contributor to the heat transfer during bubble growth. While Son et al. (1999) reported microlayer contribution in evaporation to be about 20% for a certain set of calculations. A theoretical prediction of the microlayer thickness was carried out by Zhao (2002) which focuses on individual bubbles and can be used to explain the pool boiling mechanism and to predict the heat flux in the nucleate boiling region at high heat flux and to the minimum heat flux point. Despite these efforts, studies on the effect of the microlayer are inconclusive and accurate experimental data on the thickness of the microlayer under the bubble not widely available.
2.4.4 Heat transfer overview

The mechanisms described above compete for the same heat in the liquid and hence overlap with one another, thermally speaking. At low heat fluxes characteristic of the isolated bubble region, natural convection also occurs on inactive areas of the surface, where no bubbles are growing. The rate of latent heat transport depends on the volumetric flow of vapor away from the surface per unit area.

Rohsenow (1962) proposed the first widely quoted correlation. He assumed the boiling process is dominated by the bubble agitation mechanism, whose bubble-induced forced convective heat transfer process could be correlated with the standard single-phase forced-convection correlation relation:

Mostinski (1963) applied the principle of corresponding states to the correlation of nucleate pool boiling data, arriving at a reduced pressure formulation without a surface–fluid parameter or fluid physical properties. This correlation gives reasonable results for a wide range of fluids and reduced pressures.

Stephan and Abdelsalam (1980) developed individual correlations for four classes of fluids (water, organics, refrigerants, and cryogens), utilizing a statistical multiple regression technique. These correlations used the physical properties of the fluid (evaluated at the saturation temperature) and are hence said to be physical property–based correlations.

Cooper (1984) proposed a reduced pressure expression in dimensionless form for the nucleate pool boiling heat transfer coefficient. His correlation uses reduced pressure, molecular weight, and surface roughness as the correlating parameters. Increasing the surface roughness has the effect of increasing the nucleate boiling heat transfer coefficient. The correlation covers a database of reduced pressures from 0.001 to 0.9 and molecular weights from 2 to 200 and is highly recommended for general use.

Gorenflo (1993) proposed a reduced pressure type of correlation that utilizes a fluid-specific heat transfer coefficient, defined for each fluid at the fixed reference conditions. This method is accurate over a very wide range of heat flux and pressure and is probably the most reliable of those presented. However, this approach is not extendable to boiling of mixtures, which is of interest in numerous industrial processes.

Auracher et al. (2002) and Bucholz et al. (2005), taking advantage of the growing capacities in data processing by computers in connection with miniaturized sensors and high speed cinematography and other opto-electronic facilities, conducted a series of experiments to provide a deeper insight into some of the aspects of the extremely complex mechanisms of boiling.
Chu and Yu (2009) proposed a fractal model to predict the heat transfer in nucleate boiling of a pure liquid at low to high heat fluxes including the CHF, based on the fractal distribution of nucleation sites on heating surfaces. The model presents an improved understanding of the mechanisms of nucleate pool boiling by incorporating contributions of latent heat flux, transient conduction and natural convection.

2.5 Numerical simulation

In this section, we present the different numerical methods that allow us to study the dynamics of bubble growth. First we introduce the problematic of solving of the bubble growth dynamics. We then consider the different numerical techniques allowing us to solve this dynamic problem. There are various computational methods available to solve incompressible two-phase problems. These are mainly of two types according to the mathematical representation of the liquid-vapor interface which can be either explicit or implicit. Such as the front tracking method, the boundary integral method, the volume of fluid method, the Lattice Boltzmann method, diffuse interface modelling and the level set method. Each of them has advantages and limitations. Most are limited to relatively small average or slip velocity between the two phases. We redirect our attention to the level set method and motivate this choice. In the next chapter the level set method is elaborated in detail.

2.5.1 Problems hindering modelling of boiling

Multiphase flows are often difficult to model computationally, especially because there is a steep change in physical properties such as density, viscosity etc. between one phase and the other which makes governing equations harder and the computations stiffer. Furthermore there is the difficulty of tracking the fluid-fluid interface. These are detailed below:

**Governing equations of the nucleate boiling flow:** The boiling fluid is locally either liquid or vapour. From the mathematical point of view, the two phases can be considered as a field that has two single phase regions, with moving boundaries that separate the phases. The differential equations, say the Navier-Stokes equations, hold for each of the fields separately, but cannot be applied to the whole field without violating the condition of continuity at the boundaries of each of the fields, the interface location. These boundaries, *i.e.* the geometry of the interfaces are unknown *a priori* as a function of time and space. At the interface a set of jump conditions are actually satisfied, the Rankine-Hugoniot
jump conditions. The main problematic of solving the boiling flow is thus to take into account the interface as a moving boundary. Let us now consider the mathematical representation of the interface.

**Representation of the interface location:** The location of an interface $x_i$ in a three space dimensions system can always be related to the location of a surface. The mathematical description of a surface can be either explicit, *i.e.* $x_i = f(t)$, or implicit, *i.e.* $F(x_i; t) = 0$, where $x_i$ denotes the position of the surface. This distinction is at the basis of the two families of numerical method for the solving of the boiling flows by tracking interfaces.

- The first category consists of Lagrangian methods where the interfaces are explicitly tracked throughout the simulation, meaning that the cell edges are always aligned with the interfaces (Fig 2.16a). The corresponding methods are therefore denoted explicit tracking methods.

  ![a-Explicit tracking of interface](image1.png)  ![b-Implicit tracking of interface](image2.png)

  Figure 2.16: Explicit and implicit interface representation.

- The second family consists of Eulerian interface tracking methods where the interfaces are allowed to intersect the cells arbitrarily (Fig 2.16b). This allows for fixed grids to be used which is more desirable from both computational and implementational points of view.

In the following we will present various Eulerian and Langrangian methods that have been applied to the study of two-phase flow problems.
2.5.2 Explicit tracking of interfaces

When the interface is represented explicitly, its location is tracked with the help of a moving mesh. This approach preserves a sharp interface representation but does so at the cost of introducing additional algorithmic complexities to handle break up and merging of interface segments. The governing equations also have to be modified to account for the grid movement, and periodic remeshing may be necessary if the interfaces deform too much, which may introduce additional errors.

There exists two main ways of tracking the interface dynamically.

- Either a part of the discretized elements used for describing the physical domain represents the interface, the method is either purely Lagrangian or mixed method called ALE (Arbitrary Lagrangian Eulerian).

- Or a moving additional Lagrangian grid is superposed to the fixed Eulerian grid. The resolution on the Eulerian grid must be coupled with the time dependent position of an additional Lagrangian grid which represents the interface. These are the so-called front-tracking methods.

**Lagrangian and ALE methods:** The most inconvenient feature of the purely Lagrangian methods is that the mesh becomes rapidly highly distorted. As a consequence they are to our knowledge, not applicable to the study of the liquid-vapor phase change simulations. For the second category of method, namely the ALE methods, a particular sub-element of the mesh is associated to the interface as represented on the figure below. The interface being of time dependent geometry, the mesh is distorted with time. As a consequence the governing equations need to be solved on a curvilinear moving mesh. If this method allows actually a very accurate description of the interface its numerical handling is costly and complex. Moreover the ability to take into account topological transitions as well as several bubbles is really limited.
Figure 2.17: ALE Grid

**Front-tracking method:** In the front tracking method, marker particles are explicitly introduced to keep track of the front that reduces the resolution needed to maintain accuracy. However re-gridding algorithms should be employed with front tracking method to prevent marker particles from coming together, especially at the points of larger curvature.

Figure 2.18: FTM Grid

In these methods the geometry of the interface is described with the help of a Lagrangian mesh (dots on the RHS figure) superposed on a fixed Eulerian grid, the squares in the above figure, Tryggvason *et al.* (2001). In the algorithm, the motion of the interface is an independent step of the calculation. This engenders major difficulties to apply constraints to this motion that are consistent with the main physical balances (mass, momentum, energy). The distortion of the Lagrangian mesh due to the motion of the interfaces requires to regularly reconstruct this mesh. Moreover, even though the interface is represented as a sharp surface, a necessary smearing of some source terms, like the surface tension force, must be introduced in order to insure that the solving of the governing equations on the Eulerian grid takes into account the physics of the interface. This smearing is numerically controlled and its consequences on the main balances cannot be analyzed. The topological transitions are not naturally taken into account.
2.5.3 Implicit tracking of interfaces
These add dynamics to implicit surfaces. The main idea behind interface capturing methods is to use an implicit definition of a surface to describe the interface, rather than an explicit definition. In these methods we take advantage of the fact that the phase field $F$ is not unique and only its zero isocontour determines the location of the interface. For example, the zero isocontour of $\Phi(x) = x^2 - 1$ is the is the set of all points where $\Phi(x) = 0$; i.e., it is exactly $\partial\Omega = \{-1, 1\}$. The location of the interface is only a part of the field $F$. The knowledge of the field $F$ is sufficient to capture the interface location. The corresponding methods are denoted front capturing methods.

Since the definition of $F$ can be extended to the whole two-phase system as an Eulerian field, $F$ can be numerically treated as any other physical main variable of the two-phase fluid description and there is no need to use a specific numerical discretization for the interface. This makes the numerical determination of the time dependent location of the interfaces easier.

In addition to this, coalescence and break up is, for most Eulerian methods, implicitly controlled by the grid resolution and is thus treated naturally. The drawback of using Eulerian methods is that the interfaces potentially are “smeared” across one or more cell widths requiring higher resolution and correction methods to achieve the same accuracy as for the Lagrangian methods.

In this section, we provide a short presentation of the basic ideas allowing such an interface description.

The volume of fluid method: The volume of fluid method (VOF) is based on the discretization of the volume fraction of one of the fluids. The motion of the interface is captured by solving a conservative law for volume fraction Navier-Stokes equations simultaneously. Since the interface is represented in terms of volume fraction, mass should be conserved. But certain stages of the algorithm are approximative and the conservation is inexact in most of the existing algorithms, Aulsia (2003). The VOF method needs to have accurate reconstruction algorithms to solve for the advection of volume fraction. A disadvantage of the VOF method is that it is difficult to compute accurate local curvature from volume fraction. This is due to the sharp transition in volume fraction near the interface.

Lattice Boltzmann method: The Lattice Boltzmann method is a mesoscopic approach to the numerical simulation of fluid motions based on the assumption that a fluid consists of many particles whose repeated collision, translation, and distribution converge to a state of local equilibrium yet et al. ways
remaining in flux. LBM has advantages such as implementation on a complex geometry, very efficient parallel processing, and ease of reproduction of the interface between the phases. However, LBM is not yet a widely used computational method to track the fluid motion in multiphase systems due to its computational intensity.

**Level set method (LSM):** The level set approach is another potential numerical method to solve incompressible two-phase flow incorporating surface tension term. In the level set method, the interface is represented as the zero level set of a smooth function. This has the effect of replacing the advection of physical properties with step gradients at the interface with the advection of level set function that is smooth in nature.

The level set method does not have the same conservation properties of VOF method or front tracking method. Phase leakage is an unrelenting drawback of the level set method which causes the less dense phase to leak into the denser phase, mainly when there is a steep contrast between the density and viscosity of the two interacting fluids. Phase leakage is a numerical artefact introduced by the smoothing operators at finite grid resolution. At infinitesimal grid resolution this problem would cease.

The standard remedy for phase leakage is reinitialization. In reinitialization, the thickness of the interface is maintained by iterating between time steps, an auxiliary partial differential equation is used to condition $\Phi$ to be close to a distance function from the interface, introduced by Sussman *et al.* (1994). Reinitialization is a computationally expensive workaround to re-distribute $\Phi$ to get closer to phase conservation. The problem of phase conservation is farther complicated when dealing with inter species phase change, as in the case of boiling.

The major strength of level set method lies in its ability to compute curvature of the interface easily. Furthermore level set does not require complicated front tracking regridding algorithms or VOF reconstruction algorithms. Level set method is based on continuum approach in order to represent surface tension and local curvature at the interface as a body force. This facilitates the computations in capturing any topological change due to change in surface tension.

**Diffuse interface method:** The diffuse interface method is a kindred notion to the level set method and VOF in that it computes the transport of another function that varies between the phases, the chemical or thermodynamic potential. In diffuse interface models, the interface is considered as a continuous transition zone. The main issue is then to describe the behaviour of fluid particles that are
located within the transition region. To do that, the two-phase system is first studied thermodynamically and the corresponding equations of motion are then derived.

The surface tension between two fluids is also the excess partial molar Gibbs free energy per unit surface area; so that the change of chemical potential across an interface between immiscible fluids is treated by the notion of surface tension as infinitely steep. The diffuse interface method permits this condition to be to be merely relaxed to be steep, and then a field equation for chemical potential is tracked, rather then the imposition of topology and stress balance equations implied by the notion of surface tension. The later method still requires grid adaptation, which in state of the art computational methods employ auxiliary equations for elliptic mesh generation, but are fragile in the face of topological change, e. g. coalescence or breakage phenomenon, Kolev (1993).

It is arguable whether at the same level of computational intensity; greater accuracy is assured by monitoring the free surface position using topological methods or by solving an auxiliary transport equation for a field variable. The latter method is easier to code. Of these the Level Set method is by far the most popular of the interface capturing methods, e.g. Sethian (2001).

In this method the necessary smooth extension of the main variables around the interface is made using a numerical distance function as the field $F$. To control the smearing of this field, it is regularly re-initialized. One of the difficulties of the level-set method is to ensure that the mass is actually conserved when the smearing of the distance function is such re-initialized.

### 2.6 Conclusion

Theoretically both explicit and implicit methods of interface representation can approximate the interface with the same accuracy. However, in practice that is not always achievable.

In case of the discontinuous implicit approach the indicator step-function has to be smoothed to avoid numerical oscillations, which results in an interface of finite thickness, of the order of mesh size. If we use an explicit representation this drawback is absent, and can be eliminated with the finite element version of continuous implicit approach.

In the case of changes in interface topology like merger or breakup, the explicit representation approach fails completely, and all the known remedies consist in very sophisticated ad hoc algorithms. While the implicit approaches (both continuous and discontinuous) are capable of capturing the interface independently of its topology.
These observations lead us to conclude that continuous implicit representation method combined with the finite element discretization with suitable phase correction is the best choice for numerical simulation of bubble dynamics in nucleate pool boiling.
Chapter 3
Numerical modelling

In order to model dynamic physical phenomena such as fluid flow the involved problems is posed in the form of partial differential equations based on the fundamental physical principles of continuity, momentum and energy upon which all of fluid mechanics is based. In this chapter the fundamental equations governing the dynamics of single bubbles and the associated heat transfer will be described. The liquid-vapor phase change problem involves both fluid flow and heat transfer and requires the solution of the governing equations coupled with appropriate interface boundary conditions.

The numerical results presented in this thesis required a significant amount of work to be employed in development of a moving interface program that could manage the computationally complex phenomena of bubble growth. Despite the fact that the basic concepts behind moving interfaces are rather simple, the implementation poses many practical challenges. The main purpose of this chapter is thus twofold: firstly, to describe how the code works and, secondly, to detail the schemes and numerical tricks developed to make the code reliable and accurate.

This chapter presents the computational model used in this study. The model is based on a conservative level set formulation which is used to track the interface. Isothermal flow without phase change is a special case of the formulation presented here. We write one set of transport equations valid for both phases. This local, single field formulation incorporates the effect of the interface in the equations as delta function source terms, which act only at the interface. Let us consider the mathematical representation of the interface.

3.1 Conservative level set method

This section presents the computational model used in this work to study single bubble dynamics during nucleate pool boiling. The model is based on the level set formulation of Osher and Sethian (1988). In the level set method for a two phase flow an auxiliary field the level set function \( \Phi \) is introduced to keep track of which parts of the computational domain the two phases are occupying. From a computational viewpoint, the most convenient option for choosing the implicit function \( \Phi \) is the signed normal distance to the interface. Such a variant of defining the function \( \Phi \) was advocated by A. Dervieux and F. Thomasset (1981) but fully explored and justified by Osher and Sethian (1988)
who called this method the level-set approach and the signed distance function $\Phi$ was called the level set function.

The sign of the level-set function was chosen to be ‘positive’ on one side of the interface and negative on the other, and the modulus of the function's gradient is equal to 1 everywhere (as it is a normal distance function).

The level set function $\Phi$, defined by a signed distance function $d(x)$ between a position $x$ and the interface, $\Gamma$ at time $t$ is described in the following terms:

$$d(x,t) = \text{sign} \times \min_{x,\Gamma} |x - x_i(t)|, \quad (3.1)$$

$$\phi_d = \begin{cases} 
< 0 & \text{if } x \in \text{vapor} \\
= 0 & \text{if } x \in \Gamma \\
> 0 & \text{if } x \in \text{liquid} 
\end{cases} \quad (3.2)$$

$$\Gamma_d = \{x|\phi(x,t) = 0\} \quad (3.3)$$

Where $x_i$ are the coordinates of the interface and $\text{sign}$ is positive in liquid phase and negative in vapor, using which the phase can be represented by a Heaviside function (Fig 3.1).

$$\phi_0 = HS = \begin{cases} 
-1 & \text{for } d < 0 \\
0 & \text{for } d = 0 \\
1 & \text{for } d > 0 
\end{cases} \quad (3.4)$$

The delta function $\delta(\Phi)$ is defined as the derivative of the one-dimensional Heaviside function i.e. $\delta(\Phi)=H'(\Phi)$. The delta function $\delta(\Phi)$ is identically zero everywhere except at $\delta(\Phi) = 0$.

### 3.1.1 Interface representation

Use of the Heaviside function described by Eq 3.4 has an abrupt jump at the interface and leads to poor results due to the assumed zero thickness (Fig 3.1) of the interface. Which plots of the initial level set function, the smooth level set function and the smooth delta functions for $\varepsilon = 0.01$ and with the interface centred at $d = 0$. 

51
Also, since $\delta(\Phi_0) = 0$ almost everywhere, i.e., except on the interface which has measure zero, it seems unlikely that any standard numerical approximation will give a good approximation to its integral. An alternative is to use a first-order accurate smeared-out approximation of $\delta(\Phi)$. First, the smeared-out or smooth Heaviside function $\Phi_s(d)$ needs to be defined in place of the sharp Heaviside function $\Phi_0(d)$. The smooth Heaviside function is defined as;

$$
\phi = \begin{cases} 
0 & \text{for } d < -\varepsilon \\
\frac{1}{2} \left( 1 + \frac{d}{\varepsilon} + \frac{1}{\pi} \sin \left( \frac{d \pi}{\varepsilon} \right) \right) & \text{for } -\varepsilon < d < \varepsilon \\
1 & \text{for } \varepsilon > d
\end{cases}
$$

(3.5)

Where $\varepsilon$ is a parameter that controls the interface thickness and is of the order of the average mesh element size. Then the delta function is defined as the derivative of the Heaviside function as:

$$
\delta(\phi) = \begin{cases} 
0 & \text{for } d < -\varepsilon \\
\frac{1}{2} \left( \frac{1}{\varepsilon} + \frac{1}{\varepsilon} \cos \left( \frac{d \pi}{\varepsilon} \right) \right) & \text{for } -\varepsilon < d < \varepsilon \\
1 & \text{for } \varepsilon > d
\end{cases}
$$

(3.6)

This definition of the smooth delta function and the smeared-out Heaviside function allows the surface integral to be evaluated using standard techniques such as the midpoint rule. The smooth Heaviside function and the smooth delta function are shown in Fig 3.1 along with the sharp Heaviside function. It should be noted that the smeared-out Heaviside and delta functions approach to the calculus of implicit functions leads to first order accurate methods. With the smeared-out Heaviside the errors in the calculation of integrals are $O(\Delta x)$ regardless of the accuracy of the integration.
method used. Since higher-order accurate methods can be complex, we prefer the smeared-out Heaviside and delta function methods whenever appropriate.

The smooth continuous nature of the level set function (Fig 3.2-c) which is defined at all points of the computational domain $\Omega$, makes it easy to calculate the interface normal vector and interface curvature which are obtained from the level set function gradient and the divergence of the gradient.

$$\tilde{n}_t = \frac{\nabla \phi}{|\nabla \phi|}$$  \hspace{1cm} (3.7)

$$\kappa_t = -\nabla \cdot \tilde{n}_t = -\nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right)$$  \hspace{1cm} (3.8)

To avoid the steep jump while representing physical properties across the interface resulting from Eq 3.2 Olsson et al. (2007) smear the interface over a region of width $2\varepsilon$ using a hyperbolic tangent function. Thus the level set function takes the following form.

$$\phi = \begin{cases} 
0 & \text{for } d < -\varepsilon \\
\frac{1}{2} \left( \tanh \left( \frac{2d(x)}{\varepsilon} \right) + 1 \right) & \text{for } -\varepsilon < d < \varepsilon \\
1 & \text{for } \varepsilon < d
\end{cases}$$  \hspace{1cm} (3.9)

We have chosen to represent $\phi$ by the hyperbolic tangent function. It is zero in vapor phase, unity in liquid phase and has intermediate values for the interface, $\Gamma = \{ \times | \phi(x, t) = 0.5 \}$. For example, if the interface is the circle with the centre at the origin and unit radius, the distance function can be computed as;

$$d_{r_{0}}(x, y) = \sqrt{(x^2 + y^2)} - 1$$  \hspace{1cm} (3.10)

The above equation is elaborated in Figure 3.2 which plots the unit circle centred at origin using a distance function, a Heaviside function and the hyperbolic tangent function.
Figure 3.2: Surface plot of the unit circle centred at origin at t=0 with the level set function as (a) a distance function, (b) a Heaviside function, and as (c) a hyperbolic tangent function.
3.1.2 Equation of the interface motion

We now focus on the problem of advection of the interface. The interface velocity normal to the interface direction can be found by computing the full first differential of the level set function, giving us:

\[ \vec{u}_r = \frac{\partial \phi}{\partial t} / |\nabla \phi| \]  

(3.11)

If we combine the expression for the normal interfacial velocity with the equation of continuity for fluid velocity (which is a direct consequence of mass balance) we get;

\[ \vec{u}_r = u \cdot \vec{n} \text{ on } \Gamma, \]  

(3.12)

Where \( u \) is the fluid velocity, we immediately obtain the following evolution equation for the level-set function;

\[ \frac{\partial \phi}{\partial t} + (u \cdot \vec{n}) |\nabla \phi| = 0 \text{ on } \Gamma, \]  

(3.13)

This equation is defined over the whole domain \( \Omega \), since all variables are defined there. Substituting the normal vector from (Eq 3.7) into the above expression, we derive the following pure convection equation for the level-set function \( \Phi \); that describes the evolution of \( \Phi \) corresponding to the motion of the liquid vapor interface (the \( \Phi = 0.5 \) iso-contour).

\[ \frac{\partial \phi}{\partial t} + \vec{u}_r \cdot \nabla \phi = 0 \text{ in } \Omega \]  

(3.14)

To describe the interface motion we have taken into consideration only the normal component of the interface velocity, as it should be evident in (Eq 3.12). This is a consequence of using the implicit approach for interface representation. If we relied on the explicit (parametric) representation, the interface points would be convected with fluid velocity, i.e. moving along the trajectories of fluid particles (along the characteristics); the motion of interface points would not be restricted to the normal direction. However, it is evident that only the motion of interface in its normal direction may change the interface shape; the tangential motion has no influence on the form of interface. In addition, Hou et al. (1994) and Stockie and Wetton (1999) showed: it is the tangential mode of the
interface motion that causes main stability problems. These arguments should further justify our choice of the level-set approach.

When choosing a suitable numerical method to solve Eq 3.14 one has to consider:

- The method should be conservative.
- No spurious oscillations should be introduced.
- The thickness of the interface and the profile of \( \Phi \) should remain constant.

### 3.1.3 Phase conservation

While using the advection equation (Eq 3.15) described in the previous section to transport the interface of a distance level set function we note that the profile and thickness of the interface do not remain constant. This is because when the signed distance function \( d(x,t) \) is advected by a non-uniform flow, it does not necessarily correspond to a distance function any longer. To elaborate this we consider one dimensional advection with some constant velocity.

\[
\frac{\partial \phi(x,t)}{\partial t} + \bar{u} \frac{\partial \phi(x,t)}{\partial x} = 0, \quad (3.15)
\]

Assume that initially \( d(x,t) \) is a regularized characteristic function denoted by \( d_0(x) \) that undergoes an initial perturbation \( \delta(x) \), therefore at \( t=0 \) we have;

\[
\phi(x,0) = \phi_0(x) + \delta(x), \quad (3.16)
\]

The solution to (Eq 3.14) is then;

\[
\phi(x,t) = \phi_0(x - \bar{u}t) + \delta(x - \bar{u}t), \quad (3.17)
\]

Thus the perturbations will not be dampened but simply advected with the constant velocity \( \bar{u} \).

Mulder et al. (1992) pointed out that new perturbations are constantly introduced in numerical calculations in the form of large of or small gradients of the distance level set function and therefore the shape of the profile will become more and more distorted as time evolves. It is therefore mandatory to ensure that the level set remains a distance function without changing the zero-level set, and as a consequence, researchers have focused on methods that forbid the level set function from developing large or small gradients. When this re-distancing of the level set function is performed at
the beginning of the calculation it is called initialization, and when it is performed during the computation it is called reinitialization, which is a popular way to work around the phase loss problem in the level set method.

There are many different approaches to reinitialize the level set function as a distance function:

- **Direct approach:** Chopp (1993) was the first to recognize and exploit the potential of reinitialization using a direct approach later used by Merriman (1994). It is a straightforward approach that consists in simply standing at each computational mesh point and finding the signed distance to the interface. The drawback of this approach is its computational complexity which is of the order $O(N^3)$ for an $N \times N$ grid.

- **Pseudo time approach:** This involves solving the following first order partial differential equation in pseudo-time to steady state.

$$\frac{\partial \phi}{\partial \tau} + \text{sign}(\nabla \phi - 1) = 0, \quad (3.18)$$

This was introduced by Sussman *et al.* (1994). Its virtue is that the level set function is reinitialized without explicitly finding the zero-level set. The principal drawback when solving this equation is that the zero level set, i.e., the position of the interface, might be shifted due to numerical diffusion of the underlying numerical scheme. So, even though the method does not require the localization of the interface, the computational cost of solving the nonlinear hyperbolic equation (3.19) is rather high. Moreover, any numerical scheme for the solution of (3.19) will introduce some numerical diffusion (some part of the diffusion comes also from the approximation of sign see, e.g., Sussman *et al.* (1994), which results in small inaccuracy of the interface location and some loss of mass, e.g., Tornberg (2000).

- **Fast marching method:** In order to circumvent these limitations, Sethian (1999) proposed a fast marching approach for the distance re-initialization based on locally solving the Eikonal equation $|\nabla \phi| = 1$ while employing only points closer to the interface in the numerical stencil. Fast marching methods solve the Eikonal equation
over the whole computational domain in $O(N \log N)$ operations, where $N$ is the
number of grid points in the domain. In this method a data structure is created that
allows one to march through cells in an order that permits only one pass per cell.
Using a heap sort algorithm, this procedure can be made highly efficient. However,
the accuracy of this approach is limited, and the re-distancing of the points closest to
the interface induces a displacement of the front.

In the context of multiphase flows the prominent limitations of the distance function level set
approach is that neither the level set transport nor the re-initialization inherently conserve the volume
of the region enclosed by the zero level set. For liquid-vapor flows in boiling, this can lead to gains or
losses in the mass of the liquid, which can lead to substantial errors in many applications.

In this work, we approach the problem of phase conservation by choosing a stable and accurate
numerical scheme based on finite element approach, for advecting the level set function. Instead of a
signed distance function, a hyperbolic tangent level set function $\Phi$ (Eq 3.9) has been employed which
allows us to write the advection equation (Eq 3.14) in conservative form as follows;

$$\frac{\partial \Phi}{\partial t} + \nabla \cdot (\vec{u}_\Gamma \Phi) = 0, \quad (3.19)$$

With the level set transport equation written in conservative form, and the given definition of $\Phi$, it is
clear that the scalar $\Phi$ should be a conserved quantity. As in the case of the distance level set
function, nothing insures that solving Eq. (3.18) will preserve the form of the hyperbolic tangent
profile $\Phi$. As a result, an additional re-initialization equation needs to be introduced to re-establish the
shape of the profile.

As originally proposed by Harten (1977) it is possible to add artificial compression in order to
maintain the resolution of contact discontinuities. This can be viewed as an intermediate step in
pseudo time where one is solving the conservation law:

$$\frac{\partial \phi}{\partial \tau} + \nabla \cdot f(\phi) = 0, \quad (3.20)$$

where $f$ corresponds to the compressive flux. In our case, we want the artificial compression flux to
act in regions where $0 < \phi < 1$ and in the normal direction of the interface. To achieve this, we
choose $f = \phi(1 - \phi)\hat{n}_\tau$. We denote the time variable by $\tau$ to stress that this is an artificial time, not
59
equivalent to the actual time \( t \). We note that (3.20) is a hyperbolic differential equation. As \( \tau \) increases, stationary shocks will develop at the interfaces. To avoid discontinuities at the interface, we add a small amount of viscosity or diffusive flux thus modifying the conservation law to;

\[
\frac{\partial \phi}{\partial \tau} + \nabla \cdot f(\phi) = \nabla \cdot \epsilon \nabla \phi, \tag{3.21}
\]

The diffusive flux on the right hand size of the above equation balances the normal compressive flux that aims at sharpening the profile and ensures that the profile of the liquid vapor interface remains of characteristic thickness ‘\( \epsilon \)’. Eq. 3.21 can be rewritten in conservative form, as follows;

\[
\frac{\partial \phi}{\partial \tau} + \nabla \cdot f'(\phi) = 0, \tag{3.22}
\]

Where,

\[
f'(\phi) = \nabla \cdot f(\phi) - \nabla \cdot \epsilon \nabla \phi, \tag{3.23}
\]

By solving (3.22) to steady-state the interface thickness will remain constant and proportional to \( \epsilon \). Taking advantage of the divergence free velocity field Olsson and Kreiss (2005) set the artificial time as equal to the real time in order to combine Eqs. (3.22) and (3.19) resulting in the following stabilized level set advection equation, written in conservative form:

\[
\frac{\partial \phi}{\partial t} + \nabla \cdot \left[ \hat{u} \phi + \phi(1 - \phi) \hat{u} - \epsilon \nabla \phi \right] = 0 \tag{3.24}
\]

Since both the advective as well as the reinitialization steps are formulated as conservation laws, \( \int \phi dx \) is constant in time in the continuous case. As a result, solving successively for Eq. (3.24) accomplishes the transport of the \( \Phi = 0.5 \) iso-contour, while preserving the shape of the profile and ensuring the conservation of \( \Phi \) without reinitializing the level set function at every time step.

3.1.4 Physical properties

The density and viscosity of the liquid and vapor phases is defined by scalar fields that use the level set function to distinguish between phases.
\[
\rho_{\phi} = \rho_{\gamma} + (\rho_{\gamma} - \rho_{\nu}) \phi \tag{3.25}
\]

\[
\mu_{\phi} = \mu_{\gamma} + (\mu_{\gamma} - \mu_{\nu}) \phi \tag{3.26}
\]

These are defined throughout the domain and not just on the interface, because of which a delta function is used with the curvature during numerical implementation. The delta function used (Fig 3.1) is the absolute value of the gradient of the level set function.

### 3.2 Governing equations

The level set equation is coupled to the Navier Stokes equation through the level set function and the velocity field. The Navier Stokes equation reads.

\[
\rho \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla \cdot p + \rho \vec{g} + F_s - \beta \left( T - T_{\text{sat}} \right) \vec{g} + \nabla \cdot \mu \left( \nabla \vec{u} + \nabla \vec{u}^T \right) \tag{3.27}
\]

Where the density and viscosity are given by Eq (3.25,3.26) and \( F_s \) is the local surface tension force at the interface. The surface tension forces are evaluated using the continuum surface force method of Brackbill et al. (1992).

\[
F_s = \sigma \kappa \delta_{\vec{t}} \tag{3.28}
\]

Where, \( \delta \) is the Dirac delta function localizing the surface tension force to the interface. In bubble dynamics the accurate representation of the surface tension forces is critical for the numerical model. An inaccurate calculation of these forces generates subtle spurious currents that act as parasites and contaminate the solution leading to oscillations that can be strong enough to destroy the interface Shin et al. (2005).

A proper representation of \( F_s \) should satisfy the Young-Laplace law for an interface in equilibrium. To achieve this, an important ingredient is the accurate estimation of the interface curvature. In the level set method the interface curvature can be accurately calculated since the chosen smooth Heaviside function has continuous first and second derivatives.

The continuity equation is derived by including the effects of volume expansion due to liquid-vapor phase change at the interface. Applying the chain rule we can write the continuity equation as
\[
\frac{\partial \rho}{\partial \phi} \frac{\partial \phi}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0
\]  
(3.29)

Taking \( \phi \) from Eq (3.19) where the interface velocity is given by \( \vec{u}_I = \vec{u} + \vec{u}_{ev} \).

\[
\frac{\partial \phi}{\partial t} = -\nabla \cdot \left( (\vec{u} + \vec{u}_{ev}) \phi \right)
\]  
(3.30)

And inserting into Eq (3.29) we obtain the following relation.

\[
- \frac{\partial \rho}{\partial \phi} (\vec{u} + \vec{u}_{ev}) \nabla \phi + \rho \vec{V} \vec{u} + \vec{u} \nabla \rho = 0
\]  
(3.31)

\[
\nabla \rho (-\vec{u}_{ev}) + \rho \nabla \vec{u} = 0
\]  
(3.32)

\[
\nabla \cdot \vec{u} = \frac{\vec{u}_{ev}}{\rho} \cdot \nabla \rho
\]  
(3.33)

Where the vapor velocity at the interface due to evaporation is defined in terms of the vapor mass flux and is determined by the expression:

\[
\vec{u}_{ev} = \frac{\dot{m}}{\dot{\rho}_v} \text{ where } \dot{m} = \delta \frac{\lambda \nabla T}{h_{fg}}
\]  
(3.34)

The energy equation is

\[
\rho C_p \left( \frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T \right) = \nabla \cdot \lambda \nabla T + Q
\]  
(3.35)

The computations are performed using a finite element method-based software COMSOL. The advection equation of the level set function; the incompressible Navier–Stokes equations and the energy equation are coupled with each other and are solved using the multiphysics utility. The advection equation uses the velocity field calculated using the incompressible Navier–Stokes equations plus the vapor velocity at the interface from the energy equation (Eq. 21). The dependence of the level set function in the incompressible Navier–Stokes equations comes through the physical properties as represented by Eq. (3.25, 3.26).
3.3 Contact angle

In surface science the contact angle is an important parameter as its variation may influence bubble departure diameters and growth rates during bubble growth. Sefiane et al. (1998) demonstrated that the contact angle plays a crucial role in the magnitude of the critical heat flux. Therefore, for the numerical simulation of bubble dynamics, an appropriate contact angle model is essential for a correct prediction of the bubble formation. Various approaches have been employed in literature.

3.3.1 Static contact angle approach

Because of the large uncertainties associated with determination of advancing and receding contact angles, researchers have often used a static contact angle, a constant value of the contact angle while simulating bubble dynamics during nucleate pool boiling. Son et al. (1999) assumed a static contact angle at the bubble during their numerical simulation of a single bubble on a horizontal surface during nucleate pool boiling. Their results showed that the departing bubble became larger with increase in contact angle. Abarajith and Dhir (2002) fixed the contact angle throughout the bubble growth and departure process while relating it to the Hamakar constant which was found to change with surface wettability.

A careful study of contact angle hysteresis (Eq-2.2), using drops of hydrocarbon chains was conducted by Lam et al. (2002) in order to investigate the relation between the contact angle of a liquid and the size of its molecule. The authors performed contact angle measurements of 21 liquids from two homologous series (n-alkanes and 1-alcohols) on FC-732-coated surfaces. They observed that the contact angle hysteresis decreases with the chain length of the liquid while the receding contact angle equals the advancing angle when the liquid molecules are infinitely large.

This implies that as the advancing and receding contact angles increase the hysteresis between them decreases, such that at 90° the liquid will have a constant contact angle. To elaborate this we plot the advancing and receding contact angles (ACA and RCA) measured by Lam et al. (2002) against the mean static contact angle, \( \theta_0 \) calculated from different pairs of experimentally obtained ACA and RCA given in the paper. The mean static contact angle is simply defined as the arithmetic mean between ACA and RCA, measured as:

\[
\theta_0 = \frac{\theta_{ACA} + \theta_{RCA}}{2}
\]  

(3.36)
Figure 3.3 thus demonstrates that advancing and receding contact angles become very close when extrapolated to 90°. Thus a static contact angle approach to simulating bubble dynamics is more accurate at high values of contact angle, i.e. near 90°.

Figure 3.3: Advancing and receding contact angles of n-Alkanes and 1-Alcohols versus the mean contact angle, $\theta_0$. Data from Lam et al. (2002).

### 3.3.2 Contact line velocity approach

The experimental data typically obtained for contact angle variation (e.g. Dussan 1979) in the case of a droplet is shown in Figure-3.4.
Figure 3.4: Characteristic experimental results for contact angle measurements against contact line velocity.

The contact angle is plotted as a function of contact line velocity. The fitted curve shows a quasi-linear variation of contact angle between limiting interface velocities. Here $u_{CL,\text{max}}$ denotes the limiting value of the contact line velocity at which a measurement of the contact angle was made. Based on these experimental observations the dynamic contact angle has been typically modelled as a function of the interface speed.

In the case of dynamic contact angle at the base of a vapour bubble, Ramanujapu and Dhir (1999) derived a contact angle model based on their experiments using a silicon wafer as the test surface with micromachined cavities for nucleation, during nucleate pool boiling. They calculated the interface velocity and measured the bubble base diameter as a function of time. They observed the dynamic contact angle as function of the interface velocity and obtained a figure similar to Figure-2.

Ramanujapu and Dhir (1999) found that the contact angle varied during different stages of bubble growth and was weakly dependent on the interface velocity thus the contact angle could be determined based on the sign of the interface velocity.

More recently, Mukherjee and Kandlikar (2007) studied the effects of dynamic contact angles on the formation of single bubbles during nucleate boiling using two kinds of contact line models without considering the evaporation in the microlayer. In the first approach they use a constant advancing and
constant receding contact angle depending on the sign of the contact line velocity, \( u_{CL} \) which is approximated as the rate of change of bubble base diameter.

\[
\theta_{CA} = \begin{cases} 
\theta_{ACA} & \text{if } u_{CL} \leq 0 \\
\theta_{RCA} & \text{if } u_{CL} > 0 
\end{cases}
\] (3.37)

In the second approach the dynamic contact angle is a function of the rate of change of bubble base diameter and thus contact line velocity based on Fig-3.4 with a smooth transition from receding contact angle to advancing contact angle.

\[
\theta_{CA} = \begin{cases} 
\frac{u_{CL} \left( \theta_{RCA} - \theta_{ACA} \right)}{2u_{max}} + \frac{\theta_{ACA} + \theta_{RCA}}{2} & \text{if } u_{CL} \leq -u_{max} \\
\theta_{RCA} & \text{if } -u_{max} \leq u_{CL} \leq u_{max} \\
\theta_{ACA} & \text{if } u_{CL} > u_{max}
\end{cases}
\] (3.38)

Dynamic contact angle models based on contact line velocity have been used by other researchers as well. Francois and Shyy (2003) used a method similar to one described above to simulate droplet spreading. Huang et al. (2004) computed the motion of a two-dimensional drop/bubble attached to a plane surface. For the motion of contact line and the determination of the dynamic contact angle, they used ad hoc models based on a relationship between moving contact angle and contact line speed. Smith et al. (2005) employed a contact line velocity based model to study the contact line dynamics of an interface between immiscible fluids.

One prominent aspect of the contact line velocity approach is stick-slip behaviour of the liquid vapour interface at the contact point. The change in the contact angle affects the balance of forces by altering the surface tension which acts through the contact angle. The sudden disturbance in the competing forces, the buoyancy force that pulls the bubble up and the contact line force that keeps the bubble down, causes perturbations in the liquid vapour interface, which in turn affects the velocity of contact line. This cyclic process is at the root of the stick-slip behaviour of the liquid vapour interface.

### 3.3.3 Force balance approach

In this study we implement a dynamic contact angle based on the balance between surface tension forces and buoyancy forces. It is a hypothesis that has not yet been justified in literature. In this model as well, the prescribed values of the apparent receding and the apparent advancing contact angles
define the limits of the instantaneous apparent contact angle. The transition between receding contact angle towards the advancing contact angle takes place based on the balance of buoyancy forces and surface tension forces. The underlying idea in this model is that:

- The advancing and receding contact angles are determined by the characteristics of the interaction between liquid/vapour interface and the surface, and can be determined experimentally.

- The sign of the contact line velocity is a weak indicator of the advancing/receding contact angle, Ramanujapu et al. (1999).

- The switch from RCA towards ACA can be modelled based on the ratio of the buoyancy force to the contact line force.

\[
\theta_{CA} = \begin{cases} 
\theta_{ACA} & \text{if } F_g \geq F_\sigma \\
\theta_{RCA} & \text{if } F_g \leq F_\sigma 
\end{cases}
\] (3.39)

The instantaneous shift from receding contact angle to advancing contact angle causes numerical perturbations to avoid which one can model it as a smooth transition. Thus in the force balance approach the liquid-vapor interface has the receding contact angle for a buoyancy force less than or equal to the minimum contact force, i.e. contact force in effect at receding contact angle. While the interface forms advancing contact angle with the surface when the buoyancy force is greater than or equal to the maximum contact force, i.e. contact force in effect at advancing contact angle, with intermediate values of \( \theta_{CA} \) for buoyancy force in between the minimum and maximum values.

\[
\theta_{CA} = \begin{cases} 
\theta_{ACA} & \text{if } F_g \geq F_{\sigma,max} \\
\theta_{transition} & \text{if } F_{\sigma,max} > F_g > F_{\sigma,min} \\
\theta_{RCA} & \text{if } F_{\sigma,min} \geq F_g 
\end{cases}
\] (3.40)

Instead of defining a smooth contact angle based on conditions on the force balance we can model the contact angle as a hyperbolic tangent function which will be valid throughout the simulation. This is shown as follows;
\[ \theta_{CA} = \frac{\theta_{ACA} + \theta_{RCA}}{2} + \tanh \left( \frac{F_g - F_{\sigma,\text{min}}}{F_{\sigma,\text{max}} - F_{\sigma,\text{min}}} \right) \left( \frac{\theta_{ACA} - \theta_{RCA}}{2} \right) \]  

(3.41)

Where, \( F_g \) is a function of the equivalent bubble diameter and the gravitational constant, \( g \). While \( F_{\sigma,\text{min}} \) and \( F_{\sigma,\text{max}} \) are functions of the bubble base diameter and the known values of the minimum receding contact angle and maximum advancing contact angle respectively.

### 3.3.4 Implementation of dynamic contact angle

A complication in simulating bubble growth is that the Navier–Stokes equations in combination with the no-slip boundary condition, predicts that an infinite force is required to move a contact line. Lauga (2005) present a thorough review of experimental, numerical and theoretical investigations on the subject of the fallibility of the no-slip boundary condition and existence of the slip.

Slip is said to occur when the value of the tangential component of the velocity appears to be different from that of the solid surface immediately in contact with it. Physically, there is a difference between three different types of slip:

1. Microscopic slip at the scale of individual molecules, using hydrodynamics to force liquid molecules to slip against solid molecules by involving large forces.

2. Actual continuum slip at a liquid-solid boundary (i.e., beyond a few molecular layers) and

3. Apparent (and effective) slip due to the motion over complex and heterogeneous boundaries.

The phenomenon of slip has been encountered in three different contexts. Gas flow in devices with dimensions of the mean free path of gas molecules, flow of non-newtonian fluids such as polymers and contact line motion. In the context of Newtonian liquids, solving the equations of motion with a no-slip boundary condition in the neighborhood of a moving contact line leads to the conclusion that the viscous stresses and the rate of energy dissipation have non-integrable singularities. When the singularity was explicitly formalized (Dussan and Davis 1974), it became clear that such models are physically unacceptable. To understand this it can be theorized that at the microscopic scale, surface roughness of the solid boundary produces the macroscopic slip condition which shows that at the contact line a Newtonian fluid must exhibit local slip in order to move, Davis (2003). The idea of using local slip boundary condition to remove the singularity was first suggested by Huh and Scriven.
More recently the slip boundary condition has been used by Norman and Miksis (2005) to model a gas bubble with a moving contact line rising in an inclined channel using the level set method and by Chen et al. (2009) to simulate bubble formation on orifice plates with moving contact lines using the level set method. While Afkhami et al. (2009) proposed a mesh dependent model of dynamic contact angle using local slip conditions for volume of fluid simulations.

Consequently the flow near the contact line should be modelled to allow slip locally on the fluid-solid interface. This should not be considered as a molecular slip but as an effective slip that permits the description of mathematical models which give reasonable predictions for macroscopic flow quantities. It is a device that makes the macroscopic dynamics well defined though it is also an admission that the macroscopic physics near the contact line is not well understood nor well described.

A well posed problem at the moving contact line thus requires two essential ingredients:

1. A slip law that relieves the force singularity.
2. A condition on the contact angle, $\theta_{CA}$.

The simplest slip boundary condition is the so-called free slip condition, an ad-hoc relationship valid for the entire wall;

$$\vec{n}_{wall} \cdot \vec{u} = 0$$  \hspace{1cm} (3.42)

This does not set the tangential velocity component to zero. To restrict the tangential velocity we turn to the Navier slip boundary condition (Stokes 1845) which says that there is a degree of slip at a solid boundary that depends on the magnitude of the tangential stress.

Thus at a solid wall the component $u_t$ of the fluid velocity in the direction of the unit tangent 't' is proportional to the rate of strain in that direction, the constant of proportionality ($\lambda$) being the slip length, shown in Fig 3.5.

$$\vec{u}_t = - \left( \frac{\lambda}{\mu} \right) \tau \cdot t$$  \hspace{1cm} (3.43)
Where ‘T’ is the stress vector. Therefore a zero slip length corresponds to zero tangential velocity (no-slip condition), while free slip is obtained as \( \lambda \) tends towards infinity. In our simulations, the slip length has been set equal to the mesh element size. Thus the extrapolated tangential velocity component is 0 at the distance \( \lambda \) (equal to one mesh element) from the wall, as indicated in the figure below.

![Figure 3.5: Navier-Slip boundary condition](image)

Now, a contact angle of \( \theta_{CA} \) has to be applied. This boundary condition can be expressed by the dot product between the level set normal vector at the interface and the wall normal vector;

\[
\vec{n}_{wall} \cdot \vec{n}_{T} = \cos(\theta_{CA})
\]  

(3.44)

The contact angle and slip length constraints are implemented in weak form as follows.

\[
r \left( \sigma(\tilde{n} - \cos(\theta_{CA})\tilde{n}_{T}) \delta - \tilde{u} \frac{\mu}{\lambda} \right) \tilde{u}
\]  

(3.45)

Where \( \tilde{u} \) is the test function.

### 3.4 Stability and nondimensionalization

Each interfacial flow problem is characterized by some set of non-dimensional parameters (criteria) as well as by some specific time scale. That time scale is extremely important, as it reflects the dynamics of the considered physical process; it also serves as a guideline for selecting a time-step
size in numerical simulations. Although the physical time scale is always dependent on the problem at hand, there are some common scales connected with typical physical phenomena like gravity, surface tension, viscosity.

Let \( l_R \) be the length scale of the considered problem. The gravity phenomenon is well represented by the dimensionless Froude number \( Fr = \frac{u_R}{\sqrt{gl_R}} \), where \( u_R \) is the characteristic velocity scale and \( g \) is the magnitude of the gravitational acceleration. If we denote by \( t_R \) the typical time scale of a gravity-driven physical process, then \( u_R = l_R/t_R \). A characteristic time-scale should be such that all physical effects forming corresponding non-dimensional criterion counterbalance each other; thus, from

\[
Fr = \frac{l_R}{t_R \sqrt{g l_R}} \approx 1, \tag{3.46}
\]

We can deduce

\[
t_R = \sqrt{\frac{l_R}{g}}, \tag{3.47}
\]

The surface tension phenomenon in viscous flow is characterized by the capillary number,

\( Ca = \frac{(u_R \mu)}{\sigma} \) where \( \mu \) is the dynamic viscosity and \( \sigma \) is the coefficient of surface tension. If we denote by \( t'_R \) the typical time scale for a capillarity-driven physical process, then \( u_R = l_R/t'_R \). And from stability criterion we have;

\[
Ca = \frac{l_R \mu}{t'_R \sigma} = 1, \tag{3.48}
\]

From where we deduce

\[
t'_R = \frac{l_R \mu}{\sigma}, \tag{3.49}
\]

To capture the dynamics of the modelled physical process, the numerical method should use a time-step not exceeding the time-scales of all involved physical phenomena. In bubble dynamics during nucleate pool boiling gravity driven flow is more significant than capillarity driven flow therefore we will consider the characteristic time from Eq 3.37.
3.4.1 Characteristic scales

In nucleate boiling the characteristic length is the size of the bubble when it separates from the surface. To find this dimension, we balance the bubble surface tension to the bubble buoyancy force, as shown in Fig-xx; therefore [Notes – Heat transfer with phase change (2006) pg 5/36] The length scale is of the order of bubble diameter. From which we can obtain the characteristic velocity using the characteristic time described previously.

Length scale

\[ l_R = \frac{\sigma}{g (\rho_l - \rho_v)} = 0.002497 \text{ m} \]

Characteristic time

\[ t_R = \frac{l_R}{g} = 0.015954 \text{ s} \]

Characteristic velocity

\[ u_R = \sqrt{\frac{l_R g}{\rho_l}} = 0.156508 \text{ m/s} \]

Characteristic temperature difference

\[ \Delta T = T_w - T_{sat} \]

3.4.2 Nondimensionalization

The governing equations are made dimensionless by using the characteristic scales and subsequent rescaling of the involved variables. Dimensionless numbers help to identify which physical effects are dominating, and also assist when classifying different model problems. The non dimensional quantities used to make the equations dimensionless are the Reynolds, Froude, Weber and Peclet numbers.

The governing equations, (Eqs 2.27-2.32) are nondimensionalized using the following definitions for various dimensionless quantities.

\[ t^* = \frac{t}{t_R} = \frac{u_R}{l_R} \quad x^* = \frac{x}{l_R} \quad y^* = \frac{y}{l_R} \quad u^* = \frac{u}{u_R} \quad v^* = \frac{v}{v_R} \quad \rho^* = \frac{\rho}{\rho_R} \quad \mu^* = \frac{\mu}{\mu_R} \quad p^* = \frac{p}{\rho_R u_R^2} \]

\[ T^* = \frac{T - T_{sat}}{\Delta T} \quad \lambda^* = \frac{\lambda}{\lambda_R} \quad c_p^* = \frac{c_p}{c_{pR}} \quad \kappa^* = \frac{l_R \kappa}{u_R} \quad Q^* = \frac{Q}{l_R \rho_R u_R} \]

Where the characteristic physical properties like density, viscosity and thermal conductivity etc are taken to be those of the vapor phase. Putting these definitions in Eq 3.27 we get:
\[
\begin{align*}
\rho^* \rho_R & \left( \frac{\partial \tilde{u}^*}{\partial t^*} + \frac{u_R}{l_R} \nabla \cdot \tilde{u}^* \right) + \left( \tilde{u}^* \left( \frac{u_R}{l_R} \right) \cdot \nabla \tilde{u}^* \left( \frac{u_R}{l_R} \right) \right) = -\nabla \cdot p^* \left( \frac{\rho_R u_R^2}{l_R} \right) + \frac{\sigma \delta \tilde{n}_l}{l_R^2} \\
+ \rho^* \rho_R \left( 1 - \beta_T \left( T - T_{\text{sat}} \right) \right) \tilde{g} + \nabla \cdot \mu^* \left( \frac{u_R}{l_R} \right) \left[ \nabla \tilde{u}^* \left( \frac{u_R}{l_R} \right) + \nabla \tilde{u}^* \left( \frac{u_R}{l_R} \right) \right]
\end{align*}
\]

Multiplying both sides by \( \frac{l_R}{(u_R^2 \rho_R)} \) we get:

\[
\begin{align*}
\rho^* \left( \frac{\partial \tilde{u}^*}{\partial t^*} + \tilde{u}^* \cdot \nabla \tilde{u}^* \right) &= -\nabla \cdot p^* + \left( \frac{l_R \tilde{g}}{u_R^2} \right) \rho^* \left( 1 - \beta_T \left( T - T_{\text{sat}} \right) \right) + \frac{\sigma}{\rho_R u_R^2 l_R} \kappa^* \delta \tilde{n}_l \\
+ \nabla \cdot \mu^* \left( \frac{\mu_R}{\rho_R u_R l_R} \right) \left( \nabla \tilde{u}^* + \nabla \tilde{u}^* \right)
\end{align*}
\]

Or,

\[
\begin{align*}
\rho^* \left( \frac{\partial \tilde{u}^*}{\partial t^*} + \tilde{u}^* \cdot \nabla \tilde{u}^* \right) &= -\nabla \cdot p^* + \frac{\rho^*}{Fr_R^2} \left( 1 - \beta_T \left( T - T_{\text{sat}} \right) \right) + \frac{1}{We_R} \kappa^* \delta \tilde{n}_l + \\
\frac{1}{Re_R} \nabla \cdot \mu^* \left( \nabla \tilde{u}^* + \nabla \tilde{u}^* \right)
\end{align*}
\]

Similarly the energy equation is rewritten as:

\[
\begin{align*}
\rho^* \rho_R C_p^* C_p^* \left( \frac{\Delta T}{l_R^2} \frac{\partial T^*}{\partial t^*} + \tilde{u}^* \cdot \nabla T^* \frac{\Delta T}{l_R} \right) &= \frac{1}{l_R} \nabla \cdot \lambda^* \lambda^* \nabla T^* \frac{\Delta T}{l_R} + Q^* \frac{\rho_R u_R^3}{l_R} \\
\left( \rho_R C_p \frac{\Delta T}{l_R} \frac{u_R}{l_R} \right) \rho^* C_p^* \left( \frac{\partial T^*}{\partial t^*} + \tilde{u}^* \cdot \nabla T^* \right) &= \left( \frac{\Delta T}{l_R} \lambda^* \right) \nabla \cdot \lambda^* \nabla T^* + Q^* \frac{\rho_R u_R^3}{l_R}
\end{align*}
\]

Multiplying both sides by \( l_R/(u_R C_p \rho_R \Delta T) \) we get:

\[
\begin{align*}
\rho^* C_p^* \left( \frac{\partial T^*}{\partial t^*} + \tilde{u}^* \cdot \nabla T^* \right) &= \left( \frac{\lambda^*}{\rho R C_p u_R l_R} \right) \nabla \cdot \lambda^* \nabla T^* + \left( \frac{u_R^2}{C_p^* \Delta T} \right) Q^* \\
\rho^* C_p^* \left( \frac{\partial T^*}{\partial t^*} + \tilde{u}^* \cdot \nabla T^* \right) &= \frac{1}{Pe_R} \nabla \cdot \lambda^* \nabla T^* + Ec \cdot Q^*
\end{align*}
\]

The non dimensional continuity equation is:
\[ \nabla \cdot \mathbf{u}^* = \frac{\bar{u}_{	ext{evp}}}{\rho} \cdot \nabla \rho^* \]  

(3.57)

Where,

\[ \bar{u}_{	ext{evp}} = \frac{\bar{u}_{	ext{evp}}}{u_R} \quad \text{and} \quad \dot{m} = \bar{\delta} \frac{\lambda}{h_f} \left( \frac{T^*}{T_m^*} \right) \]  

(3.58)

The level-set equation is already nondimensional.

\[ \frac{\partial \phi^*}{\partial t} + \mathbf{u}^*_i \cdot \nabla \phi^* = \nabla \cdot \left[ \varepsilon^* \left( \nabla \cdot \mathbf{n}_r \right) \mathbf{n}_r - \phi^* (1 - \phi^*) \mathbf{n}_r \right] \]  

(3.59)

### 3.5 Numerical implementation

This section describes the numerical implementation of the physical equations using COMSOL Multiphysics (formerly FEMLAB), a finite element analysis and solver utility for various physics and engineering applications, especially coupled phenomena (multiphysics). First the model is set up with the necessary approximations. Then the equations are rewritten in order to implement them in the correct form and then initial and boundary conditions are described. In the finite element method it is possible to formulate the equations and boundary conditions in strong or weak form. The strong form is what one would think of as the normal way to write the equations. The weak form is a special integral formulation of the equations that in some cases are more suited for numerical simulations. It provides the user with more possibilities to control and enforce given constraints. Nevertheless, the weak form is not as accurate as the strong form. Both forms are used to solve the present problem.

#### 3.5.1 Defining the computational domain

A vapour bubble growing on a heated surface during nucleate boiling in the absence of flow can be assumed to exhibit axially symmetric dynamics with reference to the vertical axis. As a consequence we can reduce the problem to a plane intersecting the bubble at its centre. Furthermore, one has to calculate the solution in half of the plane cutting through the centre of the bubble and the full solution for the plane can be obtained by mirroring the symmetry plane while the full spatial solution can be obtained by revolving the solution obtained for half of the intersecting plane over 360° around the
axis of symmetry. In this way the problem is reduced to two independent variables ‘r’ (radial) and ‘z’ (vertical) coordinates. The computational domain is shown in figure 3.6.

The above geometry can be drawn using the graphical user interface.

3.5.2 Implementation of the governing equations

In two dimensions the problem is solved for five fields – the level set function, the radial and vertical components of velocity, the pressure and the temperature governed by Navier stokes; level set and energy conservation equations described in the previous section.

In Comsol the governing equations are represented in the following form;

\[
d_{U_i} \frac{\partial U_i}{\partial t} + \nabla \cdot \Gamma_{U_i} = F_{U_i}, \text{ in } \Omega
\]  

(3.60)

Where the coefficient \(d_{U_i}\) and the variable vector \(U_i\) are as follows,
\[
d_{U_i} = \begin{bmatrix} \rho \\ \rho \\ 0 \\ 1 \\ \rho c_p \end{bmatrix}
\quad \text{and} \quad U = \begin{bmatrix} u \\ v \\ p \\ \phi \\ T \end{bmatrix}.
\]

The other parameters i.e. the flux tensor \( \Gamma_{U_i} \) is:

\[
\Gamma_{U_i} = \begin{bmatrix}
    r \left( p - 2 \frac{\mu_\phi}{\text{Re}_k} \frac{\partial u}{\partial r} \right) & -r \frac{\mu_\phi}{\text{Re}_k} \left( \frac{\partial u}{\partial z} + \frac{\partial v}{\partial r} \right) \\
    -r \frac{\mu_\phi}{\text{Re}_k} \left( \frac{\partial v}{\partial r} + \frac{\partial u}{\partial z} \right) & r \left( p - 2 \frac{\mu_\phi}{\text{Re}_k} \frac{\partial v}{\partial z} \right) \\
    r \phi (1 - \phi) \hat{n}_z - \epsilon \frac{\partial \phi}{\partial r} & r \phi (1 - \phi) \hat{n}_z - \epsilon \frac{\partial \phi}{\partial z} \\
    -r \frac{\lambda_\phi}{\text{Pe}_k} \frac{\partial T}{\partial r} & -r \frac{\lambda_\phi}{\text{Pe}_k} \frac{\partial T}{\partial z}
\end{bmatrix}
\]

The generalized source term \( F_{U_i} \) is:

\[
F_{U_i} = \begin{bmatrix}
p - r \left( u \frac{\partial u}{\partial r} + v \frac{\partial v}{\partial z} \right) - 2 \frac{\mu_\phi}{\text{Re}_k} \frac{u}{r} \\
\rho - \beta_\phi \Delta T - \rho \left( u \frac{\partial v}{\partial r} + v \frac{\partial u}{\partial z} \right) \\
-r \left( \frac{\partial u}{\partial r} + \frac{\partial v}{\partial z} \right) - \frac{\partial \rho}{\partial r} \left( \frac{\partial \rho}{\partial r} + \frac{\partial \rho}{\partial z} \right) \\
-r \left( \frac{\partial \phi}{\partial r} + u_{ep} n_z \hat{n}_z \frac{\partial \phi}{\partial z} + u_{ep} n_z \frac{\partial \phi}{\partial z} \right) \\
-r \rho c_p u_i \frac{\partial T}{\partial r} + \rho c_p v_i \frac{\partial T}{\partial r} - Q
\end{bmatrix}
\]

In the Comsol scripting language the above formulation is given as:

\[
equ.dim = \{ 'u', 'v', 'p', 'phi', 'T' \};
\]

\[
fem.shape = \{ 'shlag(2, ''u'' )', 'shlag(2, ''v'' )', 'shlag(1, ''p'' )', 'shlag(1, ''phi'' )', \\
'\text{shlag(2, ''T'' )}' \};
\]
equ.da = 
{{{r*rho_ns};r*rho_ns};0;\ r*Dts_phi_ls;\ r*Dts_cc*rho_cc*C_cc}});

equ.ga = 
{{{r*(-2*eta_ns*u*r+p)};\ r*eta_ns*(uz+vr)};{-*eta_ns*(vr+uz)};
'r*(-2*eta_ns*vz+p)'};{0;0};{'r*gamma*(phi*(1-phi)*nojac(normr)\ -ee*phir)'};
'r*gamma*(phi*(1-phi)*nojac(normz)\ -ee*phiz)'};{'-r*k_T_cc*Tr'};'-*k_T_cc*Tz'});

equ.f = 
{\{-r*rho_ns*(u*ur+v*uz)-2*eta_ns*u/r+p\};\ r*(F_z_ns-
 rho_ns*(u*vr+v*vz))'};
'-r*(divU_ns-usr)';\ r*(\ -u_phi_ls*phir-v_phi_ls*phiz)';\ r*(-
 rho_cc*C_cc*u_cc*Tr-rho_cc*C_cc*v_cc*Tz+Q_cc')}});

The matrix $\Gamma$ is entered in equ.ga and F in the structure equ.f. The field equ.shape defines the shape and order of the basis functions used for u, v, p, $\Phi$ and T respectively. Finally, the dependent variables are defined in equ.dim.

The force density from the surface tension term (Eq 3.64) in the Navier Stokes equation is included by taking advantage of the weak formulation

$$\frac{1}{We_k} \kappa \delta_i.$$  \hspace{1cm} (3.64)

Equation 3.63 is multiplied with a test/basis function and then integrated over the domain. This integral can be split into an integral over the domain and one over the boundary. It is the integral over the domain that defines the weak contribution. In Comsol script language this weak contribution is added as;

equ.weak = 
{\{-r*sigma*(-test(ur)*(-1+normr^2)\ -\ test(uz)*normz*normr+test(u)/r)*DELTA'};
'-r*sigma*(-test(vr)*normr*normz-test(vz)*(-1+normz^2))*DELTA';\ -\ test(divU_ns)*tauc_ns*rho_ns*divU_ns*r')};

Here ‘sigma’ is equal to the inverse of the Weber number and ‘DELTA’ has a positive non zero value only on the interface such that the integral of DELTA across the interface is always equal to one.
3.5.3 Adding the boundary conditions

The boundary conditions corresponding to the general form of Eq. (3.60) are:

\[-n_b \cdot \Gamma_{U_i} = G_{U_i} - \left( \frac{\partial R_{U_i}}{\partial U_i} \right)^T \mu_{U_i}, \text{ on } \partial\Omega \] (3.65)

\[R_{U_i} = 0, \text{ on } \partial\Omega \] (3.66)

Here \(n_b\) is the normal vector on the domain boundary. The \(\mu_{U_i}\)'s are Lagrange multipliers. These Lagrange multipliers are only relevant when the \(R_{U_i}\)'s are different from zero. More generally speaking one can create a Lagrange multiplier for each constraint the problem is subjected to. The \(R_{U_i}\) could for example be equal to one of the velocity components \(R_{U_i} = v_i\) on a specific boundary segment. This means that the x-component of the velocity must be zero on that domain boundary part. The Lagrange multiplier coefficients \(\mu_{U_i}\)'s are calculated by Comsol such that the constraint in Eq. (3.67) is fulfilled. Equation (3.66) is the Neumann condition and Eq. (3.67) is the Dirichlet condition or constraint.

The boundary constraints are given by specifying the \(R_{U_i}\) in Eq. (3.64) for each boundary segment. In the current set-up there are four boundaries denoted \(\partial\Omega_k\) for \(k = 1-4\), see Fig. 3.5. One may write:

\[R = R^{\partial\Omega_i}, \text{ for } i = 1 \rightarrow 5 \text{ and } k = 1 \rightarrow 4 \] (3.67)

Which gives a total of 20 variables. One Lagrange multiplier is introduced for \(\partial\Omega_2\) in order to enforce the contact angle condition on this boundary. This results in a weak equation on this boundary.

The first boundary, \(\partial\Omega_1\), is the symmetry boundary. The condition for symmetry is that the component of the velocity normal to the boundary, \(u\) is zero and the gradient of temperature normal to the wall is zero.

For the second boundary, \(\partial\Omega_2\), the component of the velocity normal to the wall, \(u\) has to be zero. The no-slip condition is relaxed such that the component of the velocity parallel to the wall is free. A contact angle of \(\theta_{CA}\) has to be applied according to Eq. 3.45. \(\vec{n}_{wall} \cdot \vec{n}_r = \cos(\theta_{CA})\). The weak form of which is given in Eq 3.46. No conditions are applied to the pressure and the level set function while the temperature on the second boundary is fixed at \(T_{wall}\). Boundary three, \(\partial\Omega_3\), has open boundary and a constant temperature of \(T_{sat}\). The last boundary, \(\partial\Omega_4\), has a slip boundary condition and temperature gradient normal to the wall is zero.
The temperature constraints are added using strong form while remaining constraints are implemented using the weak formulation. In Comsol scripting language the boundary conditions are simply given as:

```plaintext
bnd.ind = [1,2,3,4];

bnd.r = {0,0;0;0;'-T+T0_cc'}, {0;0;0;'-T+T0_cc'}, 0};

bnd.constr = {'-u','-u*nr_ns-v*nz_ns',0,'-u*nr_ns-v*nz_ns'};

bnd.constrf = {'test(-u)', 'test(-u*nr_ns-v*nz_ns)', 0, 'test(-u*nr_ns-v*nz_ns)'};

bnd.weak = {0, {'r*test(u)*(sigma*DELTA*(nr_ns-cos(theta)*normr)-u*eta_ns/h)'};
            {'r*test(v)*(sigma*DELTA*(nz_ns-cos(theta)*normz)-v*eta_ns/h)'}, 0, 0};
```

Here `bnd.r` defines the ‘R’ boundary. T0_cc is equal to T_wall for the second boundary and T0_cc is equal to T_sat for the third boundary. These are the only two boundaries that have strong boundary constraints. The weak constraints are defined in `bnd.constr` and the constraint force is defined in `bnd.constrf`. The contact angle is implemented through a weak force in `bnd.weak`, ‘sigma’ is equal to the inverse of the Weber number and ‘DELTA’ has a positive non zero value only on the interface such that the integral of DELTA across the interface is always equal to one.

### 3.6 Validation

To check if the implementation described above is correct we will use it on some simple configurations in order to benchmark the code. For simulation of bubble dynamics the important parameters are the surface forces on the liquid vapour interface and the computation of the flow around the bubble. We will use the derived result for the pressure in a vapour bubble to check the reliability of the code using analytical results to validate the computation of the bubble diameter.

#### 3.6.1 Static bubble in zero gravity

Our first test case is a circular bubble in static equilibrium. The net surface force should be zero, since at each point on the bubble surface the tension force is counteracted by an equal and opposite force at
79

a diametrically opposed point. A zero velocity field was observed and a pressure field that rises from a constant value of $p_{\text{out}}$ outside the bubble to a constant value of $P_{\text{in}} = P_{\text{out}} + \sigma/r_B$ inside the bubble was noted which is in accordance to the Laplace-Young law.

3.6.2 Oscillating bubble in zero gravity

A mass of fluid in a zero gravity field and a surface tension greater than zero, whose shape deviates from circular/spherical should recover the stable circular/spherical shape. The final stage of the fluid mass should have no velocity field and the pressure drop at the interface should satisfy the Young-Laplace Law.

$$
\Delta p = \frac{\sigma}{r} \text{ in 2D, and } \Delta p = 2\frac{\sigma}{r} \text{ in 3D}
$$

(3.68)

Where $r$ is the radius of circular or spherical bubble in equilibrium condition. We considered a two dimensional case using water as fluid in zero gravity conditions. This test case thus deals with the extreme conditions of 1000:1 density ratio, 100:1 viscosity ratio and a large surface tension coefficient. The initial shape of the bubble is elliptical with axis ratios of 3:2, 7:4 and 2:1 in a square computational domain of 5x5mm with triangular mesh elements. Initially the surface tension which depends on the interface curvature is greater at the narrow end of the bubble; this is shown by the vector plot in Figure 3.7. These forces compel the bubble interface to oscillate like an elastic band. Then after some time the interface comes to rest in a circular shape with a radially uniform distribution of surface tension forces. The pressure drop across the interface at the end of the simulation for the three cases is given in the following table.

<table>
<thead>
<tr>
<th>Aspect Ratio</th>
<th>Elliptical Area</th>
<th>Radius of equivalent circular bubble</th>
<th>Young-Laplace pressure drop</th>
<th>Actual pressure drop</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2:1</td>
<td>$6.280 \times 10^{-6}$</td>
<td>0.001224745</td>
<td>43.2042243</td>
<td>43.556</td>
<td>0.81421591</td>
</tr>
<tr>
<td>7:4</td>
<td>$5.495 \times 10^{-6}$</td>
<td>0.001224745</td>
<td>46.1872586</td>
<td>47.11</td>
<td>1.99782673</td>
</tr>
<tr>
<td>3:2</td>
<td>$4.710 \times 10^{-6}$</td>
<td>0.001224745</td>
<td>49.8879411</td>
<td>50.95</td>
<td>2.12888903</td>
</tr>
</tbody>
</table>

Table 3.1: Young-Laplace pressure drop across liquid vapor interface.

The percentage error in the last column is the difference between the Young-Laplace pressure drop and the calculated pressure drop as fraction of the Young-Laplace pressure drop. The overshoot in calculation can be explained due to the minor loss in vapor phase which is characteristic of the level set method caused by parasitic currents.
Figure 3.7: Relaxation of an elliptical vapor bubble of aspect ratio of 2:1 at various times with a vector plot of surface tension forces
Figure 3.8: Relaxation of an elliptical vapor bubble of aspect ratio of 7:4 at various times with a vector plot of surface tension forces
Figure 3.9: Relaxation of an elliptical vapor bubble of aspect ratio of 3:2 at various times with a vector plot of surface tension forces
Next we will examine the phase loss during the simulations and evaluate the phase conservative properties of the level set method during the dynamic process of bubble oscillation. Figure 3.10 shows the conservative properties of our model for the case of elliptical bubble with aspect ratio of 3:2. It is the difference of the initial vapor area and the integral of vapor phase over the computational domain as a fraction of the original area of vapor phase, plotted against time for the conservative and non conservative level set method.

![Figure 3.10: Relative error in area of vapor phase.](image)

The non conservative level set method shows significant phase loss which is continuously increasing due to the parasitic nature in which numerical discrepancies propagate Shin et al. (2005). The conservative level set model conserves 99% of the initial phase.
Figure 3.11: Relative error in area of vapor phase for the three aspect ratios

Note that most of the phase loss occurs at the initial stages of the computation afterwards the phase is almost entirely conserved through most of the dynamic process with only slight variations. This is more evident when we compare the areas of vapor region for the three cases, as follows:
Figure 3.12: Area of the vapor phase for the three aspect ratios

For the aspect ratio of 2:1 the interface is very dynamic throughout most of the simulation (Fig 3.7) where as the interface is less dynamic for the case of an aspect ratio of 3:2 as shown in Fig 3.9. Thus it may be said that the strong topological changes during the dynamics of vapour bubbles do not pose a threat to the phase conservative properties of the model.
Figure 3.13: Relative error in area of vapor phase for various mesh densities.

Figure 3.12 shows the mesh dependency of phase conservation. We observe that for about a 100% increase in mesh density the relative error decreases by about 1%.

3.6.3 Coalescence of vapor bubbles

In this section the conservative level set method has been applied to capture the coalescence of two vapor bubbles in a liquid column. This test permits the study of the evolution of the interface after the merging of the two bubbles allowing the assessment of the model in capturing the liquid vapour interface during extreme topological changes demonstrated by the rupture of the interface during coalescence.

Initialization: At the beginning of the simulation a 2-D axisymmetric domain is considered, with two equally sized bubbles placed at a distance of 1.5 times their diameter (Fig 3.14). The bubbles are surrounded by a liquid with the density ratio between them equal to 1:1000 the viscosity ratio is 1:10.
Figure 3.14: Initial state of the domain.

The level set function is initialized over a course of time, independent of the Navier Stokes, until the phase is uniformly conserved from one time step to the next and so on. In section 3.6.2 we noted that most of the phase loss occurs at the initial stages of the computation and afterwards the phase is almost entirely conserved. In this section we analyze the phase loss separately between the initialization of the model and the actual simulation of the dynamic problem. Figure 3.14 plots the non dimensional volume of vapor phase against the non dimensional time. We observe that some phase loss occurs during the initialization phase. However once the compressive and diffusive terms in the level set formulation are in equilibrium the phase loss stops and the volume of the vapor phase remains constant over a relatively longer period of time. Thus if the solution obtained at the end of the initialization phase, when the compressive and diffusive terms are balance, is used as the initial solution to the dynamic problem one can avoid the initial phase loss.
Figure 3.15: Phase loss during initialization of the level set function.

**Coalescence**: The rise of the two bubbles in a liquid column is captured in figure 3.16. The velocity vector field is also shown and the $\Phi = 0.5$ isocounter plots the motion of liquid-vapor interface that ultimately results in the coalescence of the two bubbles.

Figure 3.16: Coalescence of two bubbles.
The gravity driven motion of the two bubbles is captured at different time steps. Although the two bubbles are of same density and uniform size the lower bubble rises faster than the upper one because the lower bubble becomes entrapped in the wake region of the upper one and experiences its velocity field thereby reducing the effective velocity of the upper bubble. In this manner the two freely bubbles suspended in a liquid column eventually coalesce and the subsequent coalesced bubble rises again. In this way the level set method readily captures the vibrant topological changes associated with coalescence. The conservative properties of the dynamic simulation of this process are shown in figure 3.17.

![Figure 3.17: Phase loss during coalescence.](image)

We note that there are minor fluctuations in the vapor phase at the time when the bubbles coalesce this can be explained by the stretching and shrinking of the interface during the coalescence process. Once the dynamic process is complete the volume of the vapor phase stabilizes to a uniform value and we see that the vapor phase is conserved.

### 3.7 Conclusion

A conservative approach to the level set method that rules out the necessity of reinitialization, was numerically implemented to study moving interfaces. The Level Set and Navier Stokes model was tested for accuracy in the representation of liquid vapour interface, surface tension forces and phase conservation. The model was found to be robust and accurate in calculating surface tension forces across a vapor-liquid interface. The interface model was also tested to see if it could support
flexibility of the interface and it was found that the model is capable of handling topological changes involving the stretching, shrinking, rupture and rejoining during coalescence. The density and viscosity ratios for the tests were comparable to that of water and water vapour and the tests were carried out in comparison with analytical solutions. We can therefore conclude that the present model is suitable for simulation of single bubble dynamics during nucleate pool boiling.
Chapter 4
Decoupled bubble dynamics

The rate of bubble growth and the subsequent bubble motion has a tremendous influence on heat transfer. The study of bubble dynamics is a coupled problem. The rate of evaporation controls the interface speed. One approach to study bubble dynamics is to decouple the problem from energy conservation equation and use an input value of rate of evaporation. The objective is to observe how irregular evaporation rate controls bubble dynamics and the shape of bubble. As an added advantage the computational cost of simulating boiling flow is reduced by decoupling the thermal transport from the momentum and mass transport.

4.1 Growing and departing bubble

The conservative level set model described in the previous section was applied to study the dynamics of a vapor bubble growing on a horizontal surface with vapor phase injection taking place at the interface at the contact point. The bubble growth and departure process is essentially a balance of competing buoyancy forces and surface tension forces. It is therefore possible to leave out the energy transfer, for a later stage while concentrating on dynamics of a growing bubble. The vapor velocity at the interface in Eq 3.30 is chosen based on the temperature gradient required to initiate boiling, it has the following expression:

\[
\tilde{u}_{r_{L}^{*}} = (0.25 - z)\delta_t.
\] (4.1)

The expression insures a linear profile for the interface velocity (Fig 4.1), while the total evaporative vapor flux at the liquid vapour interface increases as a function of the bubble base diameter as well as local curvature by a factor of approximately 2\pi. The influence of the local phenomena at the contact line on the global dynamics of growing bubbles will be studied in section 4.2.
Accordingly the circumference of the bubble which $u_{evp}$ pushes outward begins to grow as the bubble volume increases, consequently increasing the rate of vapor phase injection and mimicking coupled bubble dynamics. Even though the rate of vapour phase injection increases, the profile of the interface velocity is still governed by Eq 4.1.

4.1.1 Effect of contact angle on bubble growth

In order to study the growth and departure of a single vapor bubble the model was solved for a contact angles, $\theta_{CA} = 50^\circ$, $\theta_{CA} = 55^\circ$ and $\theta_{CA} = 60^\circ$ while keeping a consistent velocity of the interface through Eq 4.1. It should be noted that while the velocity profile of the rate of evaporation was maintained the same in all the cases, the rate of evaporation itself was not maintained the same. If there been a condition governing the rate of evaporation for all the cases then the bubble should grow at the same rate irrespective of the contact angle. By allowing the evaporation rate to vary as a function of local dynamic conditions we were able to study the effects of the contact angle on the bubble growth.

The evolution of the bubble base diameter for the three contact angles is shown in the following figure. It is evident that the bubble lift-off time increases with the increase in contact angle. Observing the graph at reasonable amount of time after the initiation of bubble growth, i.e. $t=6$, we note that the rate of expansion of the bubble base is greater for larger contact angles.
Figure 4.2: Bubble base diameter for contact angle, $\theta_{CA} = 50^\circ$, $\theta_{CA} = 55^\circ$ and $\theta_{CA} = 60^\circ$.

However the evolution of the bubble volume for the three contact angles is quite similar, as shown in figure 4.3 which plots the equivalent bubble diameter. We note that the bubble diameter for the three cases follow a similar path for most of the initial bubble growth stage. It is only at the later stage of bubble growth when the buoyancy force is greater than the contact line force (i.e. approximately $t = 10$) that the bubble diameter for the lower contact angle falls below that of greater contact angle.

What we can deduce from these two figures is that for a given volume of vapor bubble the bubble base diameter is larger for larger contact angles because of the increase contact line force that tries to pull the bubble outward. As the contact line increases with the increase in bubble volume (until the bubble reaches departure conditions) therefore the rate of expansion of the bubble base is greater, in proportion to contact line force. In section 4.2 we will examine in more detail the interaction of local phenomena over global bubble growth dynamics.
Fig 4.4 shows the state of the vapour bubble after various intervals of time for a contact angle of 60° highlighting the initial and final stages of bubble growth and departure. In the initial stage of bubble growth the contact point moves radially outward. This horizontal movement of the bubble base is slowed down by surface tension forcing the bubble to comply with the geometric condition imposed by the contact angle. As the radial bubble growth is restricted the bubble begins to push upwards. The process of radial expansion of the bubble base and upward/outward growth of the bubble happens simultaneously and continuously. The volumetric expansion of the vapour bubble causes an increase in the buoyancy force pulling the bubble upward with respect to surface tension force which tries to hold the bubble down. The buoyancy forces are a function of the bubble volume and characterized by the bubble diameter where as the surface tension forces are characterized by the bubble base diameter.

The shape of the bubble evolves, from a small truncated sphere attached to the surface at the very beginning of our calculations, to a truncated balloon attached to the surface half way through the calculations, to a complete balloon shape just above the surface right after detachment and culminates into a mushroom shape a few millimeters away from the surface at the end of the calculation.
Figure 4.4: Bubble growth and departure pattern for a contact angle, $\theta_{CA} = 60^\circ$
The non uniform bubble motion induces a clockwise vortex in the liquid phase. When the liquid vortex becomes stronger with the increase of bubble diameter, the bubble base begins to move inwards. The inward motion of the contact point is also motivated by the increase in buoyancy force that is pulling the bubble upward. The departure process occurs very rapidly because of the dominance of buoyancy force over surface tension force accelerates as the bubble base shrinks, the bubble neck forms near the wall (Fig 4.3) and soon after that the bubble breaks off (Fig 4.3).

The small vapor portion left after the bubble has taken off serves as a nucleation point for the next bubble as the cyclic process of bubble departure during ebullition commences.

4.1.2 Bubble diameter comparison

The diameters of single bubbles and the bubble base were computed continuously throughout the growth and departure process for varying contact angles (Fig 4.5). Several theoretical relations have been proposed for predicting the size of bubbles at departure from a horizontal surface, and some of these will now be considered. Fritz (1935) was the first to develop a criterion for bubble departure based on a balance of buoyancy and surface tension forces acting on a static bubble. Based on experimental observations he proposed the following empirical expression for the bubble departure diameter:

\[ D_d = 0.0208\theta_{CA} \sqrt{\frac{\sigma}{g\left(\rho_l - \rho_v\right)}} \]  

(4.2)

Where the contact angle \( \theta_{CA} \) is measured in degrees. It has been observed that predictions of bubble diameter at departure, made from Equation (4.2) deviate from the data reported in literature, Son et al. (1999). Cole (1969) gives the following equation for bubble departure diameter as function of bubble rise velocity at departure.

\[ D_d = 0.04\theta_{CA} \left[ \frac{\sigma}{g\left(\rho_l - \rho_v\right)} \left[ \frac{g\sigma}{u_{b,d}\left(\rho_l - \rho_v\right)} \right]^{0.22} \right] \]  

(4.3)

Figure 4.5 compares the equivalent bubble departure diameter computed by our model with the ones predicted by the Fritz and Cole.
Cole’s expression was considered because it tries to take into account the dynamic effects of bubble shape, however its results deviate from the computed values as well as values predicted by Fritz at contact angle greater than 52°.

The bubble departure obtained by the correlation of Fritz (1935) is only a fraction less than the computed values which corresponds with other results found in literature. Seigel and Keshock (1964), for example found through their experiments that the Fritz correlation underestimated bubble departure diameter by a small percentage. We can therefore conclude that the decoupled model is able to accurately predict the diameter of departing vapor bubbles over a broad range of contact angles. Thus a decoupled model may be used to study the physics of bubble growth dynamics.

4.2 Local conditions and bubble growth

The dynamic aspects of the dependence of bubble growth mechanism on the local conditions near the contact line can be studied using the decoupled bubble growth model which computes dynamic growth of bubbles while simulating liquid-vapor phase change at the interface as a uniform phase injection at the contact point as a velocity term.
4.2.1 Effects of profile of the interface velocity

Here, the idea is to vary the value of the rate of uniform injection over the contact point region by varying the velocity profile while ensuring that the overall phase injection is the same. And in order to retain the vapour phase injection at a constant value we modify Eq 4.1 as follows:

\[ \tilde{u}_{\text{exp}} = \alpha (h_u - z) \delta_z \]

where \( h_u \) is the height of the velocity profile, \( \alpha \) is the ratio between the base and the perpendicular of the triangular profile of the interface velocity. The desired volume growth rate is denoted by \( \dot{V} \) and \( r_{B,b} \) is the bubble base radius. The volume growth rate \( \dot{V} \) can be chosen to be a constant or a function of another variable. In order to best mimic natural bubble growth we have chosen \( \dot{V} \) to vary as a function of time. Thus,

\[ \dot{V} = 2.25 \times 10^{-8} \sqrt{\frac{t_B}{l_e^3}} \]  

The constant term at the beginning of Eq 4.5 has units of m\(^3\)/s and is the amount of volumetric increase that the bubble be subjected at \( t=1 \)s. The characteristic time and cube of the characteristic length at the end of the equation are there to adimensionalize the rate of volumetric expansion of bubble. \( \dot{V} \) is designated as a function of the square root of time in order to resemble the non-linear behavior of volumetric expansion of vapor bubbles observed in literature.

It should be noted here that Eq 4.5 assumes continuous growth of the vapor bubble and doesn’t take into account the eventual detachment and departure of bubble from the surface. In order to incorporate bubble detachment into this model, Eq 4.5 would have to have a term that inverses the power on time \( t' \) at a given condition. However this non-trivial exercise is not necessary to study the effects local conditions on bubble growth. Therefore we retain Eq 4.5 in its current form and highlight that the validity of this simulation is limited to the period of bubble growth where the bubble base is growing outwards or until the buoyancy force is greater than the surface tension force.

This limitation still gives us the opportunity to examine variations in the bubble growth mechanism caused by the changes in the profile of the interface velocity. In order to do so, the liquid vapor
interface near the contact point was subjected to five different velocity profiles shown in table 4.1, having same rate of vapor mass increase.

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\tilde{u}_{ep}$ expression</th>
<th>Diagram</th>
</tr>
</thead>
</table>
| $\alpha = 3$ | $\tilde{u}_{ep} = 3 \left( \sqrt{\frac{2.32 \times 10^{-3}}{r_{b,b}}} - z \right) \delta_{\Gamma}$ | ![Diagram](image1)
| $\alpha = 2$ | $\tilde{u}_{ep} = 2 \left( \sqrt{\frac{3.48 \times 10^{-3}}{r_{b,b}}} - z \right) \delta_{\Gamma}$ | ![Diagram](image2)
| $\alpha = 1$ | $\tilde{u}_{ep} = \left( \sqrt{\frac{6.96 \times 10^{-3}}{r_{b,b}}} - z \right) \delta_{\Gamma}$ | ![Diagram](image3)
| $\alpha = 1/2$ | $\tilde{u}_{ep} = \frac{1}{2} \left( \sqrt{\frac{1.392 \times 10^{-2}}{r_{b,b}}} - z \right) \delta_{\Gamma}$ | ![Diagram](image4)
| $\alpha = 1/3$ | $\tilde{u}_{ep} = \frac{1}{3} \left( \sqrt{\frac{2.088 \times 10^{-2}}{r_{b,b}}} - z \right) \delta_{\Gamma}$ | ![Diagram](image5)

Table 4.1: Profiles of the applied interface velocity
While implementing the rate of evaporation, $u_{evp}$ from table 4.1, the perpendicular height of the velocity profile $h_u$ for various ratios of perpendicular to base $\alpha$, from Eq 4.4 are plotted in figure 4.5. Where as the effect of $h_u$ from Eq 4.4 on the interface velocity is visible in Figure 4.6 which shows the interface velocity for all $\alpha$’s at time = 3.

![Figure 4.5: Height of velocity profiles, $h_u$](image)

We can see from figure 4.6 that the intended velocity profile is robustly implemented. Thus the maximum interface velocity for the case $\alpha = 3$, at time = 3 in Fig 4.6-(a) is 0.47 indicating that the height of the velocity profile $h_u$ should be around 1.5. Which corresponds well with the $h_u$ indicated in figure 4.6 for $\alpha = 3$, at time = 3. Similarly there is good agreement between velocity profiles at other $\alpha$’s through out the simulation and we are assured that the idea of varying velocity profiles has been correctly implemented. We also note that the maximum velocity at the base of the bubble near the contact line for $\alpha = 1/3$ is 0.14 while for $\alpha = 3$ the maximum velocity at the contact line 0.474, showing in increase of 338%. This provides a reasonable range to study the effect of local characteristics on global dynamics of a growing bubble.
Figure 4.6: Velocity profiles, $u_{\text{exp}}$ for $\alpha=3,2,1,0.5$ and 0.33 at time $= 3$
Having scrutinized the robust local application of the rate of evaporation, we examine the evolution of the non-dimensional volumic rate of vapor injection, $\dot{V}$ versus the non-dimensional time for all cases of the vapor injection velocity profile ratio ‘$\alpha$’. This is plotted in Figure 4.8. The rate of vapor injection is by design is the same for all the cases and this is accurately concurred by the obtained graph.

![Figure 4.7: Rate of vapor injection, $\dot{V}$](image)

In the above figure while the vapor injection per unit time increases over time, the rate of increase in vapor injection decays steadily. This is designed to imitate natural bubble growth and should lead to a quasi-linear increase in the bubble volume over time, shown in figure 4.9. The volume of the bubble at the end of the simulation can be estimated by calculating the area under the curve from figure 4.8 and adding it to the initial volume of bubble. Alternatively we can integrate Eq 4.3 between the given time interval and add it to the initial bubble volume. This yields:

$$\Delta V = \int_{0}^{5} 2.25 \times 10^{-8} \sqrt{1 - \left(\frac{l_0}{l_e}\right)} \, dt = 0.35$$  \hspace{1cm} (4.6)
There is very good agreement between this estimated value of the increase in vapor volume and the volume of vapor bubble for the five cases plotted in figure 4.9.

![Graph showing volume vs. time for different values of \( \alpha \)](image)

**Figure 4.8: Non dimensional volume of vapor bubble**

The contact angle for all the test cases was kept at \( \theta_{CA} = 52^\circ \), indicating a bubble departure diameter of 0.0027m according to Eq 4.2. The equivalent bubble diameters for the calculations are shown in figure 4.10.

There is very good agreement between the bubble diameters obtained from calculations involving different values of \( \alpha \). Further more at bubble diameter at the end of the simulation is very close to the bubble departure diameter predicted by the Fritz equation (Eq 4.2). Thus the simulation covers a large part of the bubble growth process even though it was limited to the time when the bubble is growing outwards or when the buoyancy force is less than the contact line force.

So far, it has been clear that the local velocity profile at the contact line does not affect the global bubble dynamics, thus the bubble diameter continues to grow in a similar fashion despite over 300% increase in maximum bubble base velocity at the contact line.
Figure 4.9: Equivalent bubble diameter for various $\alpha$'s at $\theta_{CA} = 52^\circ$.

We now examine a characteristic more susceptible to local phenomena at bubble base, the bubble base diameter, plotted in figure 4.11. The evolution of the bubble base diameter over time for all the cases follows a similar path, there is slight variation in the exact values of the diameter that is spread out over a very small fraction of a millimeter. If we assume that the $\alpha = 1$ case provides the mean value of the bubble base diameter over the course of time, then we see that the other cases vary on both sides of the this mean path irrespective of their base to perpendicular ratio $\alpha$.

Thus while there is variation in the bubble base diameter between the different cases having different values of maximum velocity at the contact point, we can not assume that the variation in the bubble base diameter from the mean path is due entirely due to the variation in the maximum velocity at the contact point. However, we also can not completely rule out the influence of maximum contact line velocity on the bubble base diameter. It would be reasonable assume that the variation in the bubble base diameter from the mean path is more likely the result of discretization errors than the variation of maximum interface velocity near the contact point. This hypothesis is strengthened by the minute nature of the variation in bubble base diameter that is of the order of a small fraction of the mean value compared to the very large variation in the interface velocity near the contact point of the order of above 300%.
Figure 4.10: Bubble base diameter for various $\alpha$’s at $\theta_{CA} = 52^\circ$.

In consequence we can conclude that the variation of the interface velocity near the contact point does not have a significant influence on the dynamics of a growing bubble which are more dependent on the rate of evaporation.

4.2.2 Effects of the rate of evaporation

Here the rate of evaporation $\dot{V}$ is varied while the profile of the interface velocity is maintained at $\alpha = 1$. The idea is to see if the only effect of varying the rate of evaporation is to vary the speed of the dynamics of growing bubble. The rate of evaporation is varied by rewriting Eq 4.3 as:

$$\dot{V} = 2.25 \times 10^{-8} t^\alpha \left( \frac{I_R}{I_L} \right)$$

(4.7)

The change in the power of $t$ creates allows us to vary the rate of vapor phase injection as a function of time. We have considered two cases, one where $\alpha = 0.5$ as in Eq 4.3 and the second where $\alpha = 2/3$. This will increase the rate of evaporation though the change will only be prominent at higher values of $t$. The effect of this change is shown in the following figure which plots the interface velocity at $t = 3.5$. 

105
We note that the maximum interface velocity at $t = 3.5$ for the first case is $0.280$; whereas it was
$0.293$ at $t=3.5$ in the previous section (Fig 4.7-c). This is explained by the expansion of the bubble
base. A larger bubble base diameter provides the liquid vapor interface with a greater circumference
over which evaporative mass flux passes. So, in order to have the same rate of evaporation the height
of the velocity profile is diminished.

Similarly in case-II where $\dot{\alpha} = 2/3$ and the rate of evaporation is greater than the evaporative rate in
case-I where $\dot{\alpha} = 1/2$, we see that the maximum interface velocity is $0.260$ i.e. lesser than case-II. Again
this is because the bubble base has expanded more quickly due to the increased rate of evaporation.
And in order to provide the same evaporative mass flux as dictated by Eq 4.5, the height of the
interface velocity is lesser. To clarify this we next plot the bubble base diameters for the two cases.

From the following figure (4.13) it is clear that at the instant $t = 3.5$ the bubble base diameter of case-
II is greater than that of case-I and hence the difference in the maximum interface velocity.
Considering the evolution of the bubble base diameter over time, we observe that it follows the same
pattern for the two cases. At times the $\dot{\alpha} = 2/3$ curve leads, however the difference is little. To
reassure the correct implementation and resolution of the increase rate of evaporation we next plot the
volume of the vapour bubble for the two cases.
Figure 4.12: Bubble base diameter for $\alpha = 1/2$ and $\alpha = 2/3$ at $\theta_{CA} = 52^\circ$.

Figure 4.13: Volume of vapour bubble for $\alpha = 1/2$ and $\alpha = 2/3$ at $\theta_{CA} = 52^\circ$. 

Scrutinizing the evolution of bubble volume over the course of time for the two cases we note that the increase evaporation rate becomes evident at $t > 3$. Prior to that the two cases follow an almost similar path of bubble growth. Once ‘$t$’ is large enough the increased rate of evaporation manifests itself and the bubble begins to grow faster for case-II.

Overall, the only visible effect of the increased evaporation rate at the bubble base near the contact point is the quickening of the bubble growth process.

4.3 Conclusions

In this chapter we presented the idea of studying bubble dynamics independent of heat transfer. The concept was validated by comparing numerical solutions to existing widely accepted empirical solutions for the equivalent bubble departure diameter over a wide range of apparent contact angles. We then focused on the effect of local phenomena on the global dynamics of bubble growth assuming a constant angle. The maximum interface velocity at the bubble base, $u_{evp}$ near the contact point was varied by a ratio of over 300% and its effects were observed while keeping the overall rate of evaporation constant per unit of time for varying $u_{evp}$. It was noted that the local conditions have very little effect on the growth dynamics of a vapor bubble. We also elaborated the effect of the rate of evaporation in quickening the bubble growth process and its lack of influence over other aspects of the dynamics of growing bubbles.
Chapter 5
Coupled bubble dynamics

While the decoupled bubble growth model provided useful insight into the dynamics of evolving bubbles the complete numerical modelling of the single bubble growth during nucleate pool boiling requires the coupling of the thermal transport with the momentum and mass transport. In this chapter the interfacial mass transfer related with evaporation of liquid at the liquid vapor interface is implemented as a function of the temperature gradient across the interface. From which the interface velocity is calculated and used in the level set equation to displace the interface.

In the later portion of this chapter the growing bubble is endowed with a dynamic contact angle, an important characteristic of bubble dynamics, which depends on the surface and liquid properties and influences the overall heat transfer. Numerical modelling of the dynamic contact angle allows the evaluation of these effects. Another contributor to the dynamics of growing and departing bubbles is the evaporation in the microlayer. Experimental observations of the contribution of the microlayer to the overall liquid vapour evaporation have placed its influence as low as 20% to as Plesset and Prosperetti (1976), Son et al. (1999). However as shown in the previous chapter the rate of evaporation near the contact point at the bubble base has very little influence on the global dynamics of an evaporating bubble while affecting only the rate at which these dynamics take place.

Therefore keeping in mind the lack of reliable experimental data regarding the nature and contribution of the microlayer coupled with the not-too significant influence of local phenomena on global dynamics as elaborated in the previous chapter and for the sake of reducing the complexity and computational cost of the model we have not taken into account the evaporation in the microlayer. Instead the focus of this work is a robust coupling of the thermal transport with the momentum and mass transport, taking into account the effects of dynamic contact angle on bubble dynamics with the understanding that the transient conduction due to liquid motion is the major contributor to wall heat transfer during nucleate pool boiling.

5.1 Bubble growing on heated surface

The model of dynamic bubble growth is extended to include heat transfer. The heat exchange mechanisms that must be considered include heat transfer from liquid to vapor in the form of latent
heat during evaporation as well as the role of the liquid vapor interface motion in agitating the fluid and causing convection. All these phenomena that govern the heat transfer during nucleate boiling will be studied in the context of single bubble growth on a heated surface for which simulations will be carried out.

In comparison with the decoupled model exploited in the previous chapter, in this case the vapor phase transformation is a function of the temperature gradient across the interface as described in Section 3.2. The heated surface is maintained at a temperature of $T_w = T_{sat} + \Delta T$. The liquid and vapor are initially at a temperature $T_{sat}$. Because of heat loss during evaporation by the liquid phase in order to transform into vapor, the vapor phase is assumed to remain at $T_{sat}$ throughout the calculation; this is done by activating $Ec_rQ^*$ (Eq3.57) as a sink in the vapor phase that brings its temperature down to $T_{sat}$. Also a thermal boundary layer is imposed at the beginning of the simulation, the height of which is established through an initialization procedure.

### 5.1.1 Evolution of the temperature field

In this section we study the evolution of the temperature field and its influence of bubble dynamics, during the bubble growth and departure cycle for a contact angle of 54.5° and $\Delta T = 7$K. Figure 5.1 shows the initial state of the computational domain.

![Figure 5.1: Temperature field (in K) at t = 0s.](image)

Once the simulation starts the temperature gradient across the liquid vapor interface causes phase change. As a result the interface advances outwards. This pushes the liquid back and creates
convective forces which further help the heat transfer process. Figure 5.2 shows the state of the system a few instants into the simulation at real time = 0.01 seconds.

Figure 5.2: Temperature field (in K) at t = 0.01s.
We can see that the convective forces caused by the agitation of the vapor bubble are mixing the superheated liquid layer with the bulk liquid surrounding the bubble. This causes increased evaporation across as a larger area of the liquid vapor interface is now exposed to a higher temperature gradient. Thus the bubble begins to grow in a dynamic manner much the same way as decoupled bubble growth was described in section 4.2.

Figure 5.3: Temperature field (in K) at t = 0.11s.
Figure 5.3 shows the bubble at an intermediate growth stage when the bubble base diameter is near its maximum value. Soon after this point, the liquid vapor interface begins to advance towards the vapor
phase and away from the liquid. This is due to the rise of buoyancy forces that are pulling the bubble upwards in comparison with the contact line forces that are keeping the bubble down.

Figure 5.4: Temperature field (in K) at t = 0.14s.
Once the lift forces are sufficiently large the bubble departs from the heated surface. The crowding of the isotherms near the contact point at the bubble base shows that the heat flux in that region is very high (Figure 5.4). As the bubble begins to detach, these isotherms form a narrow thermal layer of super heated liquid under the bubble.

Figure 5.5: Temperature field (in K) at t = 0.16s.
The mixing effect is more pronounced when the bubble departs and the subsequent wake effects break the thermal boundary layer further distributing heat (Figure 5.4), the wake effects caused by
viscous forces also compel the bubble to adopt a mushroom like shape rather than a spherical one as visible in Fig 5.5. After the bubble rises away and colder fluid from the surrounding area fills the place vacated by the bubble, the thermal layer thickens and the isotherms relax over a greater height.

5.1.2 Progression of the flow field

The normalized flow field at the initial bubble growth stage, in and around a vapor bubble growing on a heated surface is shown in Figure 5.6. During the early period of bubble growth, the liquid around the bubble is pushed away (Fig 5.6-a). A circulatory flow pattern inside the bubble as well as in the surrounding liquid is observed (Fig 5.6-b) for the freely growing bubble.

![Figure 5.6: Normalized flow field at t = 0.0s, 0.01s and 0.11s.](image)

The vapor velocity vectors in the bubble are reflective of the bulk movement of the bubble in upward direction and the changes in the bubble shape as the bubble rises in the pool. There is no inflow or outflow of vapor at the vapor-liquid interface.

Figure 5.7 plots the normalized flow fields from the intermediate bubble growth stage to departure. At this stage the flow currents have been established in and around the bubble (Fig 5.7-a). The flow field just before bubble detachment (Fig 5.7-b) shows that the fluid is being pushed outwards on the upper portion of the bubble, whereas the liquid flow is radially inward in the lower portion of the bubble.
As the base of the bubble shrinks, a clock-wise liquid circulation is generated that draws in cooler, saturated liquid from the surroundings towards the heater surface. This circulation is proportional to the contact angle. Greater the contact angle, larger will be the velocity vectors and they will involve larger amounts of liquid. Thus the increase in bubble departure diameter with larger contact angles is also due to the increased heat flux which causes greater vapor volume growth rate.

In the previous chapter it was also observed that for uniform evaporation rate bubble departure is essentially a function of the buoyancy and surface tension forces, here we note that in the coupled model the vapor volume growth rate depends on the wall heat flux that supplies the latent heat for phase change. One is therefore able to find similar bubble dynamics by adjusting the wall heat flux to obtain an average evaporation rate that gives a vapor mass flux comparable to mass flux in the decoupled model of the previous section.

### 5.1.3 Heat transfer

The total heat flux during the growth and departure of a single bubble during nucleate pool boiling is assumed to be contributed by the following mechanisms:

- Latent heat by bubbles \( (q_{\text{LH}}) \) because of the evaporation of liquid. This was first suggested by Moore and Mesler (1961) based on their observation of rapid surface-temperature fluctuations in nucleate boiling.

- Conductive heat transfer \( (q_{\text{CON}}) \) from the heated surface to the superheated liquid layer in contact with surface.
The conductive heat transfer from this simulation will be discussed at the end of chapter in comparison with conductive heat transfer from other cases. For now we focus on the latent heat transfer produced during the stage of bubble expansion due to the vaporization of the thermal boundary layer near the liquid vapor interface. The heat flux removed by a single bubble can be obtained analytically by the following expression:

\[
q_{LH} = h_{fb} \rho_v V_B = \frac{1}{6} h_{fb} \rho_v \pi D_B^3 = 0.0117J
\]  

From the numerical simulation the latent heat flux absorbed by the evaporating bubble can be obtained by integrating the heat source term \( Q_s \) (after redimensioning it) over the computational domain and revolving it around the axis of symmetry. The total latent heat transfer can then be calculated by integrating the obtained curve over real time. This can be expressed as:

\[
q_{LH} = \int \int \Omega Q_s
\]  

The following figure shows the heat transfer from the liquid to the bubble as a function of time. The negative sign indicates that the heat is being absorbed by the bubble.

![Figure 5.8: Latent heat flux from a growing bubble.](image)
In figure 5.9 the total heat absorbed by the bubble is plotted against time.

Figure 5.9: Total heat absorbed by vapor bubble.

At the end of the simulation the total heat absorbed by the bubble is 0.0104 Joules. According to Eq 5.1, for a bubble departure diameter, \( D_b = 2.56 \text{mm} \) (from Table 5.1), the latent heat, \( Q_{LH} \) is 0.0117 Joules. There is very good agreement between the calculated latent heat transfer and the analytically known value.

### 5.1.4 Phase conservation

In this section the conservative properties of our implementation of the level set method are tested in the context of bubble growth and departure with phase change. Assessing the phase conservation properties during a dynamic process in which the amount of phase is continuously increasing is a challenging task. One way to approach this is to observe the amount phase at every time step and compare to an estimated value of the amount of that phase based on the amount of phase injection.

We accomplish this by taking observations of the volume of the vapor bubble at every instant. And by calculating the increase in vapor volume at every instant caused by the rate at which the liquid vapor interface is pulled outwards, i.e. \( u_r \). An estimate of the volume of the vapor bubble is then obtained
by integrating the rate of expansion per unit time over time thus predicting the volume of the bubble at every time step. This can be expressed as;

$$V_B = \int_\Omega \int_\Gamma u_t$$  \hspace{1cm} (5.3)

Thus, by comparing the observed and estimated volume of vapor bubble we can approximate the phase loss. In figure 5.9 the observed and estimated volume of the vapor bubble are presented.

![Figure 5.10: Phase conservation during simulation.](image)

The comparison shows good agreement up to the point where the buoyancy forces overtake the contact line forces. The overshoot in estimation of the volume of vapor bubble is caused by increments in interface velocity that are not due to evaporation but are due to the rise in buoyancy forces which influence the rate of displacement of the liquid vapor interface. Thus there is little numerical phase loss and the model is conservative during the dynamic growth of a vapor bubble with phase change.
5.2 Dynamic contact angle

In surface science the contact angle is an important parameter as its variation manipulates bubble departure diameters and growth rates during bubble growth by influencing the contact line force as well as the heat flux. Therefore, for the numerical simulation of bubble dynamics, an appropriate contact angle model is essential for a correct prediction of the bubble formation. In chapter 2, three approaches to contact angle modeling were highlighted.

- **Static contact angle approach.**

Here the apparent contact angle $\theta_{CA}$ is taken as the equivalent to the mean value of the advancing and receding contact angles.

$$
\theta_{CA} = \frac{\theta_{ACA} + \theta_{RCA}}{2}
$$

(5.4)

- **Contact line velocity approach.**

In this case $\theta_{CA}$ is a dynamic contact angle that varies as a function of contact line velocity $u_{CL}$ as defined by:

$$
\theta_{CA} = \begin{cases} 
    u_{CL} \left( \frac{\theta_{ACA} - \theta_{ACA}}{2u_{max}} \right) + \frac{\theta_{ACA} + \theta_{RCA}}{2} & \text{if } u_{CL} < -u_{max} \\
    \frac{\theta_{RCA}}{2} & \text{if } -u_{max} \leq u_{CL} \leq u_{max} \\
    \theta_{RCA} & \text{if } u_{CL} > u_{max}
\end{cases}
$$

(5.5)

Where $u_{max}$ is an input variable that decides the rate of change of the apparent contact angle from its minimum receding value to its maximum advancing value.

- **Force balance approach.**

The apparent contact angle in this case is modelled as a smooth hyperbolic tangent function of the force balance between the contact line force and the buoyancy force as defined by the following expression:

$$
\theta_{CA} = \frac{\theta_{ACA} + \theta_{RCA}}{2} + \tanh \left( \frac{F_k - F_{\sigma,\min}}{F_{\sigma,\max} - F_{\sigma,\min}} \left( \frac{\theta_{ACA} - \theta_{RCA}}{2} \right) \right)
$$

(5.6)
In this section we apply the three approaches to a single bubble growing on a heated surface during nucleate pool boiling with the minimum receding contact angle, $\theta_{RCA} = 48^\circ$, a maximum advancing contact angle, $\theta_{ACA} = 61^\circ$ and $\Delta T = 7K$.

5.2.1 Case-I: static contact angle

The results obtained from the numerical model of a single bubble growing on a heated surface with a static contact angle of $54.5^\circ$ are shown in figure 5.11.

![Figure 5.11: Approximate interface velocity (a), contact angle (b), forces acting on the bubble (c) and bubble dimensions (d) for a static mean contact angle of 54.5°.](image)
Because the interface is endowed with a thickness in the level set method exact values of the contact line velocity can not be obtained. The approximate value of the interface velocity is obtained by integrating the velocity term over the interface near the contact point and dividing by the length of the interface covered. The fluctuations in the contact line velocity are caused by discrete approach which can not accurately capture continuous phenomena. Therefore it would be difficult to model the dynamic contact angle on the basis of the contact line velocity.

By comparing Fig 5.11(a) with Fig 5.11(c) we observe that the absolute value of the interface velocity is proportional to the absolute difference between the buoyancy force and contact force. We also note that as the buoyancy force overtakes the contact force, at non-dimensional time approximately equal to 7, the interface velocity changes signs.

Thus, there is a strong relation between the balance of forces and the contact line velocity. To be more precise, the contact line velocity is inversely proportional to $F_g - F_\sigma$. Therefore it is possible to model the dynamic contact angle as function of the $F_g$ and $F_\sigma$, as in Case-III, instead of contact line velocity.

### 5.2.2 Case-II: Contact line velocity approach

A sudden change in the contact angle from the minimum receding value to the maximum advancing value causes unsteady behaviour in the bubble growth mechanism. Therefore in this case we consider a dynamic contact angle model in which the affects of the transformation of the apparent contact angle are dampened by defining the instantaneous apparent contact angle, $\theta_{CA}$ as a function of the interface velocity that changes linearly from the receding contact angle value, $\theta_{RCA}$ to the advancing contact angle value, $\theta_{ACA}$ as the interface velocity goes from a chosen positive limiting value, $u_{max}$ to a negative one, $-u_{max}$. Outside the range of the prescribed minimum/maximum contact line velocity the apparent contact angle is assigned a value of $\theta_{RCA}$ or $\theta_{ACA}$ depending on the sign of the contact line velocity, as described in Eq 5.4.

The limiting value of the interface velocity, $u_{max}$ is chosen to be 0.015m/s after considering the evolution of the interface velocity for a static contact angle of 54.5° shown in Fig 5.11(a). The results of the numerical simulation are shown in Fig 5.12.
In this case, since the contact angle is a function of the contact line velocity alone, it is sensitive to even the minute changes in the interface velocity. The interface velocity depends on the rate of expansion or contraction of bubble. Which in turn depend on many factors, including the balance of forces i.e. surface tension, bubble momentum etc. Thus, the interface behaviour is caught in a cyclic process where the interface velocity affects the contact angle and the contact angle affects the interface velocity by altering the surface tension and bubble momentum. The result of this cyclic process is visible in the fluctuation of the dynamic contact angle between $\theta_{\text{RCA}}$ and $\theta_{\text{ACA}}$ plotted in
Comparing Fig 5.11(a) and Fig 5.12(a) we note that the interface velocity drops below zero at an earlier stage, due to the decrease in the effective contact angle Fig 5.11(b) and Fig 5.12(b) which results in lesser contact force. Also at this point the contact angle changes to advancing contact angle Fig 5.12(b) and a lot of things happen simultaneously:

1. The negative interface velocity increases the contact angle to its maximal value.
2. The contact force increases due to increased contact angle.
3. The increased contact force tries to pull the bubble down thus expanding its base.
4. The expansion in bubble base increases the interface velocity to a positive value.
5. The positive value of the interface velocity reduces the contact angle to its minimal value.
6. The reduction in contact angle reduces the contact force.
7. In the absence of the increased contact force the bubble pulls upwards due to buoyancy.
8. The interface begins to move inward with a negative value of interface velocity, and the cycle restarts at step 1.

The results of this cyclic process are visible in the fluctuations in the interface velocity, Fig 5.12(a). In the pulsating contact angle Fig 5.12(b). In the variation of the contact force Fig 5.12(c) and in the levelling of the bubble base diameter in Fig 5.12(d). This behaviour is more a result of the brutal/sudden nature of the numerical implementation of the dynamic contact angle and is computationally exhaustive.

The force balance near the contact point influences the ability of the bubble base to expand or contract, inducing the slip/stick behaviour described in the previous case. Dussan (1979) explains slip/stick behaviour as when the motion of a contact line appears to be unsteady and spasmatic when the contact angle is changing below a certain smallest reported speed. Beyond this range the contact line movement ought to be smooth. However we note that the contact angle is oscillating continuously leading to a solution that is computationally expensive and shows pronounced slip/stick behaviour of the contact line.
We also note that despite the fluctuation in the contact line velocity and the contact angle the buoyancy and contact line force curves are quite similar for both Case-I and Case-II. In both cases the maximum and minimum values of buoyancy force and the contact line force are roughly the same and the buoyancy over takes the contact line force at about the same time, \((t = 6)\). This shows that the force balance is take a lot of influence from the fluctuations in the contact angle or contact line velocity due to slip/stick behaviour and motivates the modelling of the dynamic contact angle based on a force balance approach.

Figure 5.13: Approximate interface velocity (a), dynamic contact angle (b), forces acting on the bubble (c) and bubble dimensions (d) for an apparent contact angle as a function of the force balance.
5.2.3 Case-III: Force balance approach

Numerical calculations are carried out with the apparent instantaneous contact angle at the bubble base obtained as a function of the force balance between buoyancy force and the contact line force, caused by evaporative mass flux and surface tension respectively, according to Eq. 5.5. The results for obtained for the apparent contact line velocity, the contact angle and the force balance and bubble dimensions are plotted in Fig 5.13.

Comparing $F_g$ and $F_\sigma$ between the three cases, we note that the buoyancy force, $F_g$ overtakes the contact force $F_\sigma$ at a slightly later time for Case-III, Fig 5.13(c), this is because as the buoyancy force tries to cross the contact line force the contact angle begins to change from minimum receding value towards maximum advancing value 5.13(b). This in turn tries to bubble base outwards causing an increase in the bubble base diameter, Fig 5.13(d). This causes an increase in the contact line force which is responsible for the delay in the buoyancy force crossing over the contact line force.

We not that as the contact angle changes from $\theta_{RCA}$ to $\theta_{ACA}$ the interface velocity changes signs, Fig 5.13(a). The slip/stick behaviour at the beginning and intermediate stages of bubble growth stops as soon as the liquid-vapor interface reaches $\theta_{ACA}$ and keeps it. At around the same time the bubble base diameter shows a marked increase in rate of expansion.

5.2.4 Comparison with experimental data

Ramanujapu and Dhir (1999) experimentally studied the dynamic contact angle at the base of a vapor bubble growing on a horizontal surface during nucleate pool boiling of deionized water, using a silicon wafer as the test surface with micro-machined cavities for nucleation. They measured the bubble base diameter and apparent contact angle as a function of time and argued that the dynamic contact angle could be modelled as a function of the interface velocity even though the variation of the contact angle with interface velocity seemed to be weak because they observed a trend in the contact angle dependency on the sign of the interface velocity. During their experiments the contact angle was found to vary between $48^\circ$-$61^\circ$ for $\Delta T = 7K$, which corresponds to our test case. Figure 5.14 shows their results for the measurement of apparent contact angle calculated from experimentally obtained still images and plotted as a function of time.
Figure 5.14: Contact angle vs time for $\Delta T = 7K$, from Ramanujapu and Dhir (1999)

The advancing and receding fronts clearly vary between 48° and 61°, while the mean angle between them is about 54° which corresponds to the static contact angle of the liquid on the surface at the base of a droplet, measured by the authors just prior to the commencement of the boiling experiment. The experimentally observed evolution of the apparent contact angle over time resembles that of Case-III with a forced balance approach to modelling the dynamic contact angle. In both cases the transition from receding contact angle to advancing contact angle is smooth.

Next, the progression of the bubble diameter obtained from the same experiments by Ramanujapu and Dhir (1999) is shown in Figure 5.15. Each bubble diameter curve begins at the point of bubble nucleation and ends when the bubble departs from the heater surface, the three curves correspond to three successive bubble growth cycles. Variation in the bubble departure diameter between the three cycles is minor.
The following table summarizes the results of the four studies (three numerical and one experimental) of the dynamic contact angle and its effects on the dynamics of a single bubble growing on a heated surface during nucleate pool boiling. There is excellent agreement between the experimentally observed bubble departure diameter and the bubble departure diameter obtained by numerical simulation using a force balance model for the dynamic contact angle, Case-III.

<table>
<thead>
<tr>
<th></th>
<th>Diameter [mm]</th>
<th>Time [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case I</td>
<td>2.56</td>
<td>0.151</td>
</tr>
<tr>
<td>Case II</td>
<td>2.65</td>
<td>0.167</td>
</tr>
<tr>
<td>Case III</td>
<td>2.80</td>
<td>0.178</td>
</tr>
<tr>
<td>Experimental Results</td>
<td>2.82</td>
<td>0.042</td>
</tr>
</tbody>
</table>

Table 5.1: Bubble characteristic at departure for various test cases.
However there is considerable difference in bubble departure time between the experimental and numerical studies. This is due to the absence of a microlayer evaporation model as explained at the beginning of the chapter. The close agreement between the bubble departure diameters verifies our assertion that the rate of evaporation near the contact point at the bubble base has little influence on the global dynamics of an evaporating bubble while affecting the rate at which these dynamics take place.

Now focusing on the results obtained from the three different cases of numerical simulations we observe that departure diameter and time are slightly smaller for the case of the static contact angle. Thus the use of static contact angle will under-predict the bubble departure diameter and time. In case II it is clear that during the transitory period the contact angle will have an approximately mean value. This is also evident from Fig 5.12(b).

Thus choosing contact line velocity approach to model dynamic contact angle diminishes the advantages of a dynamic contact angle model and the model resembles a static mean contact angle approach. It is also evident from Eq 5.2 that a choice of a very low $u_{\text{max}}$ would resemble a constant advancing and constant receding contact angle approach. This would explain the slight inaccuracy of contact line approach of modelling dynamic contact angles in predicting bubble departure characteristics.

### 5.2.5 Heat transfer comparison

The heat absorbed by the system during the transformation from the liquid to the vapor phase for the three cases of dynamic contact angle approaches, i.e. static contact angle, contact line velocity based dynamic contact angle and force balance based dynamic contact angle is shown in figure 5.16.

While the conductive heat transfer from the heated surface to the superheated liquid just above it, for the three cases is plotted in figure 5.17. From both these plots the effect of the contact angle on heat transfer during the dynamic growth of a single in nucleate pool boiling is quite evident.
Figure 5.16: Latent heat transfer for different contact angle models.

Figure 5.17: Conductive heat transfer for different contact angle models.
In the case of the static mean contact angle, the both the conductive and latent heats are high at the beginning since the static mean contact angle of 54.5° is greater than the receding contact angle 48°. However at the end of the simulation the heat transfer for the static contact angle is less as the mean contact angle is less than the advancing contact angle, 68°. Thus the plots show that the heat transfer is proportional to the contact angle.

5.3 Conclusion

Heat transfer mechanisms at the local scale of a bubble growing on a heated surface have been highlighted. These mechanisms consist of the absorption of heat available at the heater surface by the liquid in the thermal boundary layer and its transport through natural convection. This heat is transferred to vapor phase as latent heat during evaporation. Once the vapor bubble begins to grow, its agitation causes convective forces that further mix the fluid and help transfer heat from superheated liquid in layer to the surrounding liquid. This thermal mixing is increased at bubble departure when wake effects break the thermal boundary layer causing additional heat distribution.

The influence of a dynamic apparent contact angle on the dynamics of a single vapor bubble nucleating on a heated wall were included in the numerical simulation considering different approaches of contact angle at the bubble base. The static mean contact angle model based on the maximum advancing and minimum receding contact angle is the simplest to implement but under predicts the bubble departure characteristics. Modeling the dynamic contact angle as a function of the contact line velocity requires a robust estimation of the velocity of the liquid vapor interface that is endowed with a thickness in the level set method. This approach is susceptible to discretization errors and over pronounced stick/slip behavior leading to loss of accuracy in the determination of bubble departure characteristics. The force balance approach provides an excellent alternative to modeling dynamic contact angles with the most accurate results for bubble departure characteristics. However, inorder to completely predict bubble dynamics over time the microlayer evaporation needs to be taken into account though the absence of microlayer evaporation provides qualitative and, in certain cases, quantative data regarding bubble dynamics.
Chapter 6
Concluding remarks

This study was undertaken recognizing the need to have more physics based approach to the understanding of boiling heat transfer that is based on the underlying physical mechanisms and is more reliable than the existing, predominantly empirical approach. The focus of the work was the nucleate pool boiling process at the macroscopic level with the objective to numerically simulate the dynamics of single bubble growing on heated surface during nucleate pool boiling at the macroscopic scale. The work can roughly be divided into two categories or stages:

• Development of level set model to simulate bubble dynamics
• Application of the model to the study of bubble dynamics.

The relative accomplishments made against these two objectives are summarized in the following section.

6.1 Advances made in this work

A conservative level set method was applied to the study of bubble dynamics. This liberates the user from the computational cost associated with reinitialization techniques previously used to limit phase loss during the utilization of the level set method. The numerical model thus obtained was found to be robust and efficient. Further more it is flexible and can therefore be used to study different kinds of fluids or fluid combinations in system where axial symmetry can be assumed. Further more the use of commercially available solver for the implementation ensures its compatibility and facilitates its extension.

The validated model was used to study the effects of local phenomena on global dynamics of a growing bubble in the context of a decoupled approach. This approach permitted the study of interface dynamics independent of the thermal transport that causes it. Through this model the local conditions near the contact point were demonstrated to have very little effect on the growth dynamics of a vapor bubble. The effect of the rate of evaporation in quickening the bubble growth process was elaborated and its lack of influence over other aspects of the dynamics of growing bubbles was highlighted.
Next, the level set and Navier Stokes model was coupled to the energy equation to study the dynamics of bubble growth in correlation with the associated heat transfer. The effects of wall heat flux on bubble dynamics has been the subject of many studies in the past. In this work our focus has been on exploring the implementation of a conservative level set approach, without reinitialization to the study of bubble dynamics at the macroscale level.

A force-balance approach to the modeling of a dynamic apparent contact angle, based on the physics of the moving contact line dynamics, was proposed in this study. It was tested against the traditional contact line velocity approach of modeling dynamic contact angle which mimics actual physics as experimental data indicates a weak relationship between contact line velocity and contact angle. The force-balance approach was validated in comparison to experimental data available in the literature. This approach reduces the non-physical stick/slip behavior of the contact line in comparison to the contact line velocity model, and allows a smooth transition from the minimum receding contact angle to the maximum advancing contact angle which is more akin to the physical phenomena. The affects of the dynamic contact angle on heat transfer were also observed. It was demonstrated that the heat transfer during bubble growth in nucleate pool boiling is proportional to the apparent contact angle.

6.2 Publications during PhD studies

- Peer reviewed research papers

- Peer reviewed conference proceedings
6.3 Outlook

The focus of this work has been the study of bubble dynamics at the macroscale level by exploiting a conservative level set approach, without reinitialization. The next step will be to include the contribution of the interacting sub-processes while moving towards a complete numerical simulation of bubble dynamics and the associated heat transfer processes. Most important, is the need to account for evaporation in the liquid microlayer. Once that is done a complete three dimensional numerical simulation can be targeted with flow conditions in order to respond to a wider range of industrial applications.

The model that has been developed in the work is very flexible and generic and allows for the inclusion of many interesting physical phenomena such as micro gravity, multi body coalescence etc. Thus another possibility is to use the current model to study other multiphase phenomena at the macroscopic scale besides boiling, like droplet dynamics.


70. Rayleigh, Lord. (1917). On the pressure developed in a liquid during the collapse of a spherical cavity. Phil. Mag. 34, 94-98.


Appendix A

Comsol scripting code

% COMSOL Multiphysics Model M-file
% Generated by COMSOL 3.5a (COMSOL 3.5.0.603, $Date: 2008/12/03 17:02:19$)
% Some geometry objects are stored in a separate file.
% The name of this file is given by the variable 'flbinaryfile'.

flclear fem

% COMSOL version
clear vrsn
vrsn.name = 'COMSOL 3.5';
vrsn.ext = 'a';
vrsn.major = 0;
vrsn.build = 603;
vrsn.rcs = '$Name: $';
vrsn.date = '$Date: 2008/12/03 17:02:19 $';
fem.version = vrsn;

flbinaryfile='1 NS LS HT DCA Fsg dT7 - t12p0 TBL.mphm';

% Constants
fem.const = {
'rho_l', '958[kg/m^3]', ...
'rho_v', '0.59[kg/m^3]', ...
'miu_l', '0.2818e-3[Pa*s]', ...
'miu_v', '0.0125e-3[Pa*s]', ...
'g', '9.81[m/s^2]', ...
'sig', '0.0611[N/m]', ...
'a', '0.0003/10', ...
'b', '0.0003/10', ...
'gam', '1', ...
'ee', '0.047', ...
'cc', '0.5', ...
'CA0', 'rca', ...
'10', 'sqrt(sig/(g*(rho_l-rho_v)))', ...
'u0', 'sqrt(g*10)', ...
'Re0', 'rho_R*10*u0/miu_R', ...
'Fr0', 'u0/sqrt(g*10)', ...
'We0', 'rho_R*u0^2*10/sig', ...
'sigm', '1/We0', ...
'tt0', '5*ee/gam', ...
'cp_v', '1889.2', ...
'cp_l', '4279', ...
'k_v', '0', ...
'k_l', '0.679', ...
'h1', '2.2606e6', ...
'Tsat', '373.15[K]', ...
'q', '1e5[W/m^2]', ...
};
'p_atm','101325[Pa]', ...
't0', '10/u0', ...
'Tw', 'Tsat+dT', ...
'Tsat0', '(Tsat-Tsat)/(Tw-Tsat)', ...
'Tw0', '(Tw-Tsat)/(Tw-Tsat)', ...
'Pe0', '10*u0*rho_R*cp_R/k_R', ...
'R0', '(a+b)*0.5*cos(CA0)', ...
'rho_R', '0.5*(rho_v+rho_l)', ...
'miu_R', '0.5*(miu_v+miu_l)', ...
'k_R', 'k_l', ...
'cp_R', '0.5*(cp_v+cp_l)', ...
'dT', '7', ...
'rca', '48*pi/180', ...
'aca', '61*pi/180', ...
'u_clmx', '0.02'};

% Geometry

clear draw
g4=flbinary('g4','draw',flbinaryfile);
draw.s.objs = {g4};
draw.s.name = {'R1'};
draw.s.tags = {'g4'};
fem.draw = draw;
fem.geom = geomcsg(fem);
fem.mesh = flbinary('m1','mesh',flbinaryfile);

% (Default values are not included)

clear appl  
appl.mode.class = 'NavierStokes';
appl.mode.type = 'axi';
appl.name = 'ns';
appl.module = 'CHEM';
appl.gporder = {4,2};
appl.cporder = {2,1};
appl.assignsuffix = '_ns';
clear prop  
clear weakconstr  
weakconstr.value = 'off';
weakconstr.dim = {'lm1','lm2','lm3','lm4','lm5','lm6','lm7','lm8','lmpsi'};
prop.weakconstr = weakconstr;
appl.prop = prop;
clear bnd  
bnd.symtype = {'ax','sym','sym'};
bnd.type = {'sym','walltype','open'};
bnd.walltype = {'noslip','slip','noslip'};
bnd.ind = [1,2,3,2];
appl.bnd = bnd;
clear equ  
equ.eta = 'eta';
equ.gporder = {1;1;2});
equ.rho = 'rho'0';
equ.cporder = {{1;1;2}};
equ.cdon = 0;
equ.sigma = 0;
equ.F_z = 'Fz';
equ.epsilon = 'hmax_ns';
equ.ind = [1];
appl.equ = equ;
fem.appl(1) = appl;

% Application mode 2
clear appl
appl.mode.class = 'ConvDiff';
appl.mode.type = 'axi';
appl.dim = {'phi'};
appl.name = 'ls';
appl.module = 'CHEM';
appl.assignsuffix = '_ls';
clear prop
clear weakconstr
weakconstr.value = 'off';
weakconstr.dim = {'lm9'};
prop.weakconstr = weakconstr;
appl.prop = prop;
clear bnd
bnd.type = {'ax','Nc'};
bnd.ind = [1,2,2,2];
appl.bnd = bnd;
clear equ
equ.D = 0;
equ.init = 'phi0';
equ.v = 'v+uint*normz';
equ.u = 'u+uint*normr';
equ.name = 'default';
equ.ind = [1];
appl.equ = equ;
fem.appl(2) = appl;

% Application mode 3
clear appl
appl.mode.class = 'ConvCond';
appl.mode.type = 'axi';
appl.name = 'cc';
appl.module = 'CHEM';
appl.assignsuffix = '_cc';
clear prop
clear weakconstr
weakconstr.value = 'off';
weakconstr.dim = {'lm10'};
prop.weakconstr = weakconstr;
appl.prop = prop;
clear bnd
bnd.type = {'qc','ax','T','T'};
142

bnd.T0 = {0,0,'Tw0','Ts0'};
bnd.ind = [2,3,4,1];
appl.bnd = bnd;
clear equ
equ.C = 'cp0';
equ.Q = 'Qs';
equ.sdtype = 'supg';
equ.rho = 'rho0';
equ.sdif = 'off';
equ.init = 'Ts0';
equ.k = 'kappa';
equ.v = 'v*(phi>cc)';
equ.u = 'u*(phi>cc)';
equ.ind = [1];
appl.equ = equ;
fem.app[3] = appl;
fem.sdim = ['r','z'];
fem.frame = ('ref');

% Shape functions
fem.shape =
{'shlag(2,''u''),'shlag(2,''v''),'shlag(1,''p''),'shlag(2,''phi''),'shlag(2,''T'')};

% Integration order
fem.gporder = {4,2};

% Constraint order
fem.cporder = {2,1};
fem.border = 1;

% Equation form
fem.form = 'general';

% Subdomain settings
clear equ
equ.cporder = {{1;1;2;1;1}};
equ.f = {{'r*rho_ns*(u*ur+v*uz)-2*eta_ns*u/r+p','r*(F_z_ns-
     rho_ns*(u*vr+v*vz))','r*(divU_ns-usource)';
     'r*(-u_phi_ls*phir-v_phi_ls*phiz)';
     'r*(-rho_cc*C_cc*u_cc*Tr-rho_cc*C_cc*v_cc*Tz+Q_cc)'});
equ.da =
{{'r*rho_ns';'r*rho_ns';0;'r*Dts_phi_ls';'r*Ds_cc*rho_cc*C_cc'});
equ.c =
{{'r-2*eta_ns*ur+pr,ur';'-r*eta_ns*uz+vr,ur';
     'r*rho_ns*(uz+vr),vr';
     '-d{r*eta_ns*(uz+vr),uz}',
     '-d(r*eta_ns*(uz+vr),uz)',
     '-d(r*(-2*eta_ns*ur+p),ur)',
     '-d(r*(-2*eta_ns*ur+p),uz)'},
     '-d(r*(-2*eta_ns*ur+p),vr)',
     '-d(r*(-2*eta_ns*ur+p),uz)',
     '-d{r*(2*eta_ns*ur+p),pr}',...
     '-d{r*eta_ns*(uz+vr),pr}',
     '-d{r*eta_ns*(uz+vr),pz}',
     '-d{r*eta_ns*(uz+vr),pz}',
     '-d{r*eta_ns*(uz+vr),pz}'}};
\input{equations}

\begin{equation}
\begin{aligned}
\{ -d(r*(-2*eta_ns*ur+p),\phiir); -d(r*(-2*eta_ns*ur+p),phiz); -d(-r*eta_ns*(uz+vr),\phiir), -d(-r*eta_ns*(uz+vr),phiz); -d(-r*eta_ns*(vr+uz),ur), -d(-r*eta_ns*(vr+uz),uz); -d(-r*eta_ns*(vr+uz),\phiir), -d(-r*eta_ns*(vr+uz),phiz); -d(-r*eta_ns*(vr+uz),Tr), -d(-r*eta_ns*(vr+uz),Tz); -d(r*(-2*eta_ns*vz+p),ur), -d(r*(-2*eta_ns*vz+p),uz); -d(r*(-2*eta_ns*vz+p),\phiir), -d(r*(-2*eta_ns*vz+p),phiz); -d(r*(-2*eta_ns*vz+p),Tr), -d(r*(-2*eta_ns*vz+p),Tz); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),ur); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),uz); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),vr); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),vz); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),pr); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),pz); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),phir); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),phiz); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),Tr); -d(-r*gamma*(phi*(1-phi)*nojac(normr)-ee*phir),Tz); -d(r*k_T_cc*Tr,ur), -d(r*k_T_cc*Tr,uz), -d(r*k_T_cc*Tr,vr), -d(r*k_T_cc*Tr,vz), -d(r*k_T_cc*Tr,pr), -d(r*k_T_cc*Tr,pz), -d(r*k_T_cc*Tr,phir), -d(r*k_T_cc*Tr,phiz), -d(-r*k_T_cc*Tr,Tr), -d(-r*k_T_cc*Tr,Tz); -d(-r*roh_ns*(u*ur+v*uz)+2*eta_ns*u/r+p,u), -d(-r*roh_ns*(u*ur+v*uz)+2*eta_ns*u/r+p,u), -d(r*k_T_cc*Tr,Tr), -d(r*k_T_cc*Tr,Tz); -d(-r*k_T_cc*Tr,Tr), -d(-r*k_T_cc*Tr,Tz); -d(-r*k_T_cc*Tr,Tr), -d(-r*k_T_cc*Tr,Tz) \}; \end{aligned}
\end{equation}
' - d\{r \* rho_{ns} \* (u \* ur + v \* uz) - 2 \* eta_{ns} \* u / r, p, phi \}, ... 
' - d\{r \* rho_{ns} \* (u \* ur + v \* uz) - 2 \* eta_{ns} \* u / r, T \}, ... 
' - d\{r (F_{z ns} - rho_{ns} \* (u \* vr + v \* vz)), u \}, ... 
' - d\{r (F_{z ns} - rho_{ns} \* (u \* vr + v \* vz)), v \}, ... 
' - d\{r (F_{z ns} - rho_{ns} \* (u \* vr + v \* vz)), phi \}, ... 
' - d\{r (F_{z ns} - rho_{ns} \* (u \* vr + v \* vz)), T \}; ... 
' - d\{-r \* (divU_{ns} + usource), u \}, ... 
' - d\{-r \* (divU_{ns} + usource), v \}, ... 
' - d\{-r \* (divU_{ns} + usource), p \}, ... 
' - d\{-r \* (divU_{ns} + usource), phi \}, ... 
' - d\{-r \* (divU_{ns} + usource), T \}; ... 
' - d\{r \* (-eta_{ns} \* ur + p), u \}, ... 
' - d\{r \* (-eta_{ns} \* ur + p), v \}, ... 
' - d\{r \* (-eta_{ns} \* ur + p), phi \}, ... 
' - d\{r \* (-eta_{ns} \* ur + p), T \}; ... 
' - d\{-r \* (2 * eta_{ns} * vz + p), u \}; ... 
' - d\{-r \* (2 * eta_{ns} * vz + p), v \}; ... 
' - d\{-r \* (2 * eta_{ns} * vz + p), phi \}; ... 
' - d\{-r \* (2 * eta_{ns} * vz + p), T \}; ... 
' - d\{-r \* (2 * eta_{ns} * vz + p), u \}, ... 
' - d\{-r \* (2 * eta_{ns} * vz + p), v \}, ... 
' - d\{-r \* (2 * eta_{ns} * vz + p), phi \}, ... 
' - d\{-r \* (2 * eta_{ns} * vz + p), T \}; ... 
' - d\{-r \* gamma \* (phi * (1 - phi) * nojac(normr) - ee * phir), u \}; ... 
' - d\{-r \* gamma \* (phi * (1 - phi) * nojac(normr) - ee * phir), v \}; ... 
' - d\{-r \* gamma \* (phi * (1 - phi) * nojac(normr) - ee * phir), phi \}; ... 
' - d\{-r \* gamma \* (phi * (1 - phi) * nojac(normr) - ee * phir), T \}; ... 
...
\begin{align*}
\text{equ.gporder} &= \{(1;1;2;1;1)\}; \\
\text{equ.weak} &= \{\{r\cdot\sigma\cdot(-\text{test}(ur)\cdot(-1+\text{normr}^2) - \\
&\text{test}(uz)\cdot\text{normz}\cdot\text{test}(ur)\cdot(-1+\text{normr}^2))\cdot\Delta\}; \\
\text{equ.be} &= \{\{\text{divU}_n\cdot\text{tau_c}_n\cdot\text{rho}_n\cdot\text{divU}_n\cdot r\}; \\
&\{\text{divU}_n\cdot\text{tau_c}_n\cdot\text{rho}_n\cdot\text{divU}_n\}, \{\text{divU}_n\cdot\text{tau_c}_n\cdot\text{rho}_n\cdot\text{divU}_n\cdot v\}; \\
&\{\text{divU}_n\cdot\text{tau_c}_n\cdot\text{rho}_n\cdot\text{divU}_n\cdot p\}; \\
&\{\text{divU}_n\cdot\text{tau_c}_n\cdot\text{rho}_n\cdot\text{divU}_n\cdot \text{phi}\}; \\
&\{\text{divU}_n\cdot\text{tau_c}_n\cdot\text{rho}_n\cdot\text{divU}_n\cdot T\}; \\
&\{\text{divU}_n\cdot\text{tau_c}_n\cdot\text{rho}_n\cdot\text{divU}_n\cdot \text{Tr}\}; \} \\
\end{align*}
'\[-d(r*(-\rho_{cc}\*C_{cc}\*u_{cc}\*Tr-\rho_{cc}\*C_{cc}\*v_{cc}\*Tz+Q_{cc}),pz)\},'\[-d(r*(-\rho_{cc}\*C_{cc}\*u_{cc}\*Tr-\rho_{cc}\*C_{cc}\*v_{cc}\*Tz+Q_{cc}),phir)\];
...'
'\[-d(r*(-\rho_{cc}\*C_{cc}\*u_{cc}\*Tr-\rho_{cc}\*C_{cc}\*v_{cc}\*Tz+Q_{cc}),phiz)\},'\[-d(r*(-\rho_{cc}\*C_{cc}\*u_{cc}\*Tr-\rho_{cc}\*C_{cc}\*v_{cc}\*Tz+Q_{cc}),Tr)\];
...'
'\[-d(r*(-\rho_{cc}\*C_{cc}\*u_{cc}\*Tr-\rho_{cc}\*C_{cc}\*v_{cc}\*Tz+Q_{cc}),Tz)\})\];
equ.ind = [1];
equ.dim = {'u','v','p','phi','T'};
equ.var = {'U_ns','sqrt(u^2+v^2)',
...'
'V_ns','uz-vr',
...'
divU_ns','ur+vz+u/r',
...'
cellRe_ns','rho_{ns}*U_{ns}*h/eta_{ns}',
...'
res_u_ns','r*(rho_{ns}*(ut+u*r+u*vz)+pr-F_{r_ns})+2*eta_{ns}*(u/r-ur)-eta_{ns}*[2*urr+uzv+vrz]',
...'
res_v_ns','r*(rho_{ns}*(vt+u*r+vz)+pz-F_{z_ns})-eta_{ns}*[r*(vrr+uzr)+2*r*vzz+uz+vr]',
...'

\tau mum_ns','nojac(min(timestep/rho_{ns},0.5*h/max(rho_{ns}*U_{ns},6*eta_{ns}/h)))',
...'
\tauc_ns','nojac(0.5*U_{ns}*h*min(1,rho_{ns}*U_{ns}*h/eta_{ns}))',
...'
res_p_ns','rho_{ns}*U_{ns}*h/eta_{ns}',
...'
gradphi_r_l_s','phir',
...'
dfluxphi_r_l_s','-Drrphi_l_s*phir-Drphi_l_s*phiz',
...'
cfluxphi_r_l_s','phi*u phi_l_s',
...'
tfluxphi_r_l_s','dfluxphi_r_l_s+cfluxphi_r_l_s',
...'
gradphi_z_l_s','phiz',
...'
dfluxphi_z_l_s','-Dzrphi_l_s*phir-Dzphi_l_s*phiz',
...'
cfluxphi_z_l_s','phi*v phi_l_s',
...'
tfluxphi_z_l_s','dfluxphi_z_l_s+cfluxphi_z_l_s',
...'

beta phi_r_l_s','r*u phi_l_s',
...'
beta phi_z_l_s','r*v phi_l_s',
...'

res phi_l_s','r*(Drrphi_l_s*phir+Drphi_l_s*phiz)',
...'
res sc phi_l_s','r*(phir*u phi_l_s+phiz*v phi_l_s-R phi_l_s)',
...'
da phi_l_s','r*Dtsphi_l_s',
...'

\grad T_r_cc','Tr',
...'
d flux T_r_cc','-krr T_cc*Tr-krz T_cc*Tz',
...'
c flux T_r_cc','rho_{cc}*C_{cc}*u_{cc}*Tr',
...'
tflux T_r_cc','dflux T_r_cc+cflux T_r_cc+sdflux T_r_cc',
...'
\grad T_z_cc','Tz',
...'
d flux T_z_cc','-kzr T_cc*Tr-kzz T_cc*Tz',
...
'cflux_T_z_cc', 'rho_T_cc*C_T_cc*T*v_T_cc', ...
'tflux_T_z_cc', 'dflux_T_z_cc+cflux_T_z_cc+sdflux_T_z_cc', ...
'beta_T_r_cc', 'r*rho_T_cc*C_T_cc*u_T_cc', ...
'beta_T_z_cc', 'r*rho_T_cc*C_T_cc*v_T_cc', ...
'grad_T_cc', 'sqrt(grad_T_r_cc^2+grad_T_z_cc^2)', ...
'dflux_T_cc', 'sqrt(dflux_T_r_cc^2+dflux_T_z_cc^2)', ...
'cflux_T_cc', 'sqrt(cflux_T_r_cc^2+cflux_T_z_cc^2)', ...
'tflux_T_cc', 'sqrt(tfux_T_r_cc^2+tflux_T_z_cc^2)', ...
'cellPe_T_cc', 'h*sqrt(beta_T_r_cc^2+beta_T_z_cc^2)/Dm_T_cc', ...
'kmean_T_cc', 'k_cc', ...
'tauet_T_cc', '0', ...
'helem_T_cc', 'h', ...
'Dm_T_cc', 'r*rho_T_cc^2*C_T_cc^2*(krr_T_cc*u_T_cc^2+krz_T_cc*u_T_cc*v_T_cc+
kzr_T_cc*v_T_cc^2)/((rho_T_cc*C_T_cc*u_T_cc)^2+(rho_T_cc*C_T_cc*v_T_cc)^2+eps)', ...
'tauem_T_cc', 'r*(-krr_T_cc*Trr-krz_T_cc*Trz+Tr*rho_T_cc*C_T_cc*u_T_cc-
kzr_T_cc*Trz+kzz_T_cc*Tvz+Tv*rho_T_cc*C_T_cc*v_T_cc-Q_T_cc)', ...
'da_T_cc', 'r*Dts_T_cc*rho_T_cc*C_T_cc', 'rho_ns', 'rho0', ...
'eta_ns', 'eta', ...
'F_r_ns', '0', ...
'F_z_ns', 'Fz', ...
'F_phi_ns', '0', ...
'eta0_ns', '1', ...
'n_ns', '0', ...
'lambda_ns', '0', ...
'eta_inf_ns', '0', ...
'type_visc_ns', 'power', ...
'kappadv_ns', '0', ...
'rhoadvns_ns', '0', ...
'rhoencns_ns', '0', ...
'epsilonp_ns', '1', ...
'Q_ns', '0', ...
'brinkmaneqns_ns', '0', ...
'delid_ns', '0.5', ...
'delds_ns', '0.25', ...
'cdtype_ns', 'sc', ...
'deldc_ns', '0.35', ...
'delps_ns', '1', ...
'ck_ns', '0.1', ...
'impression_ns', '0', ...
'usedElement_ns', 'Lagp2p1', ...
'finestMCellen_ns', 'Lagp2p1', ...
'gls_ns', '0', ...
test(nojac(rho_ns))*(nojac(u)*ur+nojac(v)*uz)+pr+2*nojac(eta_ns)*(u/r-
ur)/r-nojac(eta_ns)*(2*urr+uzz+vrz))*taum_ns*res_u_ns-
test(nojac(rho_ns))*(nojac(v)*vr+nojac(v)*vz)+pz-
nojac(eta_ns)*((urr+uzr^2+vzz+(uz+vr)/r))*taum_ns*res_v_ns-
test(divU_ns)*tauc_ns*res_p_ns', ...
'gijgij_ns', '0', ...
'usedelem_1s_ns', 'Lagp2p1', ...
'rhol1_ns', '1', ...
'rho2_ns',1, ...  
'eta1_ns',1, ...  
'eta2_ns',1, ...  
'sigma_ns',0, ...  
'gamma_ns',1, ...  
'chi_ns',1, ...  
'epsilon_ns',hmax_ns', ...  
'dfdphi_ns',0, ...  
'kappabr_ns',1, ...  
'U_ref_ns','U_ns', ...  
'D_phi_ls',0, ...  
'Dr_phi_ls',0, ...  
'Dzr_phi_ls',0, ...  
'Drz_phi_ls',0, ...  
'Dzz_phi_ls',0, ...  
'Dts_phi_ls',1, ...  
'u_phi_ls','u*uint*normr', ...  
'v_phi_ls','v*uint*normr', ...  
'K_phi_ls',0, ...  
'k_cc','kappa', ...  
'Dts_cc',1, ...  
'rho_cc','rho0', ...  
'C_cc','cp0', ...  
'Q_cc','Qs', ...  
'fluidtype_cc','userdefined', ...  
'ptype_cc','gauge', ...  
pgaugeref_cc',101325, ...  
p_cc',0, ...  
'QpworkOn_cc',0, ...  
'QviscOn_cc',0, ...  
'eta_cc',0, ...  
'etaT_cc',0, ...  
'Rs_cc',287, ...  
'Mn_cc',0, ...  
'u_cc','u*(phi>cc)', ...  
'v_cc','v*(phi>cc)', ...  
'usedElement_cc','Lag2', ...  
'finestMCell_em_cc','Lag2', ...  
'idon_cc',0, ...  
'delid_cc',0.5, ...  
'sdon_cc',0, ...  
'sdtype_cc','supg', ...  
'delsd_cc',0.25, ...  
'cdon_cc',0, ...  
'glim_cc','0.01[K]/helem_T_cc', ...  
'gamma_cc',1, ...  
'sdiff_cc','off', ...  
'kT_cc',0, ...  
'krr_T_cc','kappa', ...  
'kzz_T_cc','kappa', ...
% Interior mesh boundary settings
equ.bnd.gporder = {{1;1;2;1;1}};
equ.bnd.ind = [1];
fem.equ = equ;

% Boundary settings
clear bnd
bnd.cporder = {{1;1;2;1;1}};
bnd.shape = [1;2;3;4;5];
bnd.h = {0;0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
'omega0_ns', 10, ...
'Uref_ns', 1, ...
'LT_ns', 0.01, ...
'IT_ns', 0.05, ...
'dw_ns', '0.5*h', ...
'dwplus_ns', 100, ...
'U0_ns', 0, ...
'V0_ns', 0, ...
'p0_entr_ns', 0, ...
'Lentr_ns', 1, ...
'p0_exit_ns', 0, ...
'Lexit_ns', 1, ...
'phi0_ns', 0, ...
'Vf0_ns', 0, ...
'theta_ns', '0.5*pi', ...
'beta_ns', 'h', ...
'nr_ns', 'nr', ...
'nz_ns', 'nz', ...
'Fbndr_ns', 0, ...
'Fbndz_ns', 0, ...
'd_ls', 1, ...
'nr_ls', 'nr', ...
'nz_ls', 'nz', ...
'N_phi_ls', 0, ...
'c0_phi_ls', 0, ...
'Dbnd_phi_ls', 0, ...
'q0_cc', 0, ...
'T0_cc', {0,'Tw0','Tsat0',0}, ...
'kbnd_cc', 0, ...
'd_cc', 1, ...
'nr_cc', 'nr', ...
'nz_cc', 'nz', ...
'N_T_cc', 0, ...
'c0_T_cc', {0,'Tw0','Tsat0',0},

fem.bnd = bnd;

% Scalar expressions
fem.expr = {'gphi', 'sqrt(phir^2+phiz^2+eps)', 'DELTA', 'gphi', ...
'rho', 'rho_v+(rho_l-rho_v)*phi', ...
'miu', 'miu_v+(miu_l-miu_v)*phi', ...
'Fz', '-rho0/Fr0^2', ...
'normr', 'phir/(gphi+eps)', ...
'normz', 'phi/(gphi+eps)', ...
'int0', '((r^2/a^2)+((z-R0)^2/b^2)-1)', ...
'phi0', '0.5*(tanh(0.5*int0/ee)+1)', ...
'rho0', 'rho/rho_R', ...
'miu0', 'miu/miu_R', ...
'p1', 'p*u0*u0*rho_R', ...
'gamma', 'gam', ...
'ub', 'ubl/a_v0', ...
'uint', 'mdot/(rho_v*u0)', ...
'k', 'k_v+(k_l-k_v)*(phi>cc)', ...

150
'cp', 'cp_v+(cp_l-cp_v)*phi', ...
'k0', 'k/k_R', ...
'cp0', 'cp/cp_R', ...
'T1', 'T*dT+Tsat', ...
'mdot', 'DEL*k_l*dT^gT/(hl*10)', ...
'usource', 'uint*grho/rho_ns', ...
'grho', 'sqrt(d(rho_ns,r)^2+d(rho_ns,z)^2+eps)', ...
'DEL', 'gphi*dee'*((gphi*dee)>0.1)', ...
'Qs', '-T*(phi<cc)*300', ...
'gT', 'sqrt(Tr^2+Tz^2+eps)', ...
'sigma', 'sigm*(z<2)', ...
'eta', 'miu0/nojac(Re0)', ...
'rho0', 'NonDimensional Density', ...
'Fz', '-(rho0-betaT*(T1-Tsat))/Fr0^2', ...
'phi0', 'flc2hs(int0,4*ee)', ...

% Descriptions
clear descr
descr.expr = {'eta', 'miu0/nojac(Re0)', 'rho0', 'NonDimensional Dynamic Viscosity', 'p1', 'Dimensional pressure', 'usource', 'mdot*(rho_l-rho_v)gphi+phi0/(rho_v*rho_ns)', 'rho0', 'NonDimensional Density', 'Fz', '-(rho0-betaT*Tsat)/Fr0^2', 'phi0', 'flc2hs(int0,4*ee)', 'k', '0+k_l*(phi>cc)', 'uint', '0.5*(t>2.75)*(0.25-z)*(z<0.25)*DELTA'};
fem descr = descr;

% Coupling variable elements
clear elemcpl
% Integration coupling variables
clear elem
elem.elem = 'elcplscalar';
elem.g = {'1'};
src = cell(1,1);
clear bnd
bnd.expr = {{},{'2*pi*r*(phi<=cc)'},{}},{{},{'2*pi*r*sig*DEL'},{}},...
{'tflux_T_z_cc'},{{},{}},{{},{'tflux_T_z_cc'}},{{},{}},{{},{}},{{},{}},{{},{}},...

bnd.ipoints = {{},{}},
bnd.frame = {{},{}},
bnd.ind = {{},{}},
clear equ
equ.expr = {{},{}},{{},{}},{'1*(phi<=cc)'},{'p1*(phi<=cc)'},{'1*(phi<cc)'},

'p1*(phi>cc)',{'U_ns*(phi<=cc)'},{'2*pi*r*(phi<cc)'},
'1*(phi<=cc)*(gphi>1)*(z<2.25)',{'res_T_cc'},{'Qs'},

'2*pi*r*(uint*normr)*(uint>0)*rho_v'};
'2*pi*r*(v+uint*normz)*(uint>0)*rho_v', { ... 
'u*(z>0.01)*(z<=0.1)*(phi>0.46)*(phi<=0.54)', { ... 
'(z>0.01)*(z<=0.1)*(phi>0.46)*(phi<=0.54)'))

equ.ipoints = 
{{},{},{},{},{4},{4},{4},{4},{4},{4},{4},{4},{4},{4},{4}};

equ.frame = 
{{},{},{},{},{ref},{ref},{ref},{ref},{ref},{ref},{ref},{ref}};

equ.ind = {{{1}}};

tc{1} = {{},bnd,equ};

elem = tc; 
geomdim = cell(1,1); 
geomdim{l} = {();

elem.geomdim = geomdim; 
elem.var = {'a_bb','Fsig','HT0','HT1','a_v0','p_v0','a_10','p_10','ub1', ...
     'vb_0','A2','rdT','dHT','mdt1_lr_v','mdt1_lz_v','u_c10','c10');

elem.global = 
{{1},{2},{3},{4},{5},{6},{7},{8},{9},{10},{11},{12},{13},{14}, ...
    '15',{16},{17}};

elem.maxvars = {}; 
elemcpl{l} = elem; 
felemcpl{l} = elemcpl;

% Global expressions 

tc.globalexpr = {'dp','(p_v/a_v)-(p_l-a_l)' ...
    'dv','100*vb_0/(0.93*(4/3)*pi*a^3)', ...
    'mass','mas0*l0^3', ...
    'x','r*10', ...
    'y','z*10', ...
    'a_v','a_v0*l0*10', ...
    'a_l','a_l0*l0*10', ...
    'p_v','p_v0*l0*10', ...
    'p_l','p_l0*l0*10', ...
    'bbD','2*sqrt(a_bb*l0*10/pi)', ...
    'bD','(6*vb_0*l0*10/100/pi)^(1/3)', ...
    'Fsig','Fsig0*l0*sin(theta0)', ...
    'Fsigma','Fsig*l0*sin(rca)', ...
    'Fsig0','Fsig0*l0*sin(rca)', ...
    'theta0','0.5*(theta0+theta1)*tanh((Fbuoy-Fsig0)/(Fsig1-Fsig0+eps))', ...

152
% Descriptions
descr = fem.descr;
descr.const = {'rho_v', '1', 'We0', 'Weber', 'k_l', '@ 100°C', 'k_R', '0.5*(k_v+k_l)', 'Re0', 'Reynolds', 'cp_l', '@ 100°C', 'miu_l', '1.04e-3 [Pa*s]', 'h_l', 'latent heat of vaporisation 2.260e6 [J/kg]', 'Fr0', 'Frouds', 'q', 'inward heat flux', 'cp_v', '@ 100°C', 'rho_l', '1000', 'gam', '1/u0', 'k_v', '@ 100°C 0.025', 'miu_v', '1.3e-5 [Pa*s]', 'p_atm', 'Atm pressure', 'CA0', 'Initial Contact Angle 0.5*(rca+aca)', 'cc', 'Interface iso-contour 0 or 0.5');
fem.descr = descr;

% ODE Settings
clear ode
clear units;
units.basesystem = 'SI';
ode.units = units;
fem.ode=ode;

% Multiphysics
fem=multiphysics(fem, ...
    'bdl',[1,3,4], ...
    'sdl',[]);

% Extend mesh
fem.xmesh=meshextend(fem, ...
    'dofversion',1);

% Retrieve solution
fem.sol=flbinary('sol1','solution',flbinaryfile);

% Save current fem structure for restart purposes
fem0=fem;