Microscopic modelling of boiling

A thesis by

Giovanni Giustini

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Abstract

One of the main thermal-hydraulic challenges of LWR modelling is the prediction of boiling phenomena.

This thesis describes numerical and analytical studies aimed at modelling the heat transfer and hydrodynamics of a single steam bubble during nucleate boiling of water, aiming both to improve our current understanding of the phenomena - of the evaporation process itself, and of nucleate boiling heat transfer - and to improve our ability to predict such phenomena, at both single bubble and component scales.

Analytical and CFD studies of bubble formation are described. These require accurate representations of evaporation from the liquid microlayer at the bubble base. This vaporization has been investigated from a molecular point of view, with modelling based on kinetic theory, and an apparent inconsistency in measurements of microlayer evaporation during bubble formation has been resolved, and an improved understanding of the molecular mechanism of phase-change thereby gained. The importance of including this improved representation of the evaporation process in single-bubble CFD simulations has been demonstrated.

Aiming to improve the closure relations employed for component-scale CFD simulation of boiling flows, interface-tracking modelling of bubble growth and release has been used. Single-bubble interface-tracking models have been developed in an attempt to quantify the transient conduction (“quenching”) component of nucleate boiling heat transfer, associated with bubble lift-off. These mechanistic models allowed detailed quantification of the complex physics associated with bubble growth, and with quenching of the dry area at the bubble base that takes place at bubble departure. A large discrepancy was observed between estimates of the quench heat transfer from these interface-tracking simulations, and that incorporated in the more approximate modelling embodied in the closure relations widely used in component scale CFD.
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Declaration of originality

This thesis describes the author’s own work. The work of other authors is referenced as such.

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This thesis is dedicated to my Mother and my Father.
What is now proved was once only imagin’d

William Blake – ‘Proverbs of Hell’
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LIST OF SYMBOLS

Latin:

c, specific heat capacity [J/Kg/K]

C, microlayer slope, dimensionless

d, thickness [m]

D, bubble diameter

f, evaporation coefficient, dimensionless

f, body force vector [N/m³]

F, signed distance function [m]

h, heat transfer coefficient [W/m²/K]

hfg, latent heat of evaporation [J/Kg]

H, Heaviside step function, dimensionless

k = 1.38×10⁻²³ [J/K], Boltzmann constant

l, characteristic length [m]

m, mass [Kg]

Θ, molar mass [g/mol]

n, time level, dimensionless

n, unit vector normal to a surface, dimensionless

N, number of (molecules, nucleation sites)

NA = 6.023×10²³ [mol⁻¹], Avogadro’s number

p, pressure [N/m²]

q, heat [J]

q, heat flux vector [W/m²]

r, radial distance [m]
\( R \), bubble radius [m] 

\( R_g = 8.314 \text{ [J/mol/K]}, \) universal gas constant 

\( \mathcal{R} = R_g/R \), specific gas constant [J/Kg/K] 

\( s \), slope, dimensionless 

\( S \), surface area [m²] 

\( t \), time [s] 

\( T \), temperature [K] or [°C] 

\( \mathbf{u} \), velocity vector [m/s] 

\( v \), rewet velocity 

\( V \), volume [m³] 

\((x,y,z)\), spatial coordinates in Cartesian geometry [m] 

\((NX,NY,NZ)\) number of mesh cells along \((x,y,z)\) directions 

**Greek:** 

\( \alpha = \frac{1}{\rho c} \), thermal diffusivity \([m^2/s]\) 

\( \beta \), growth constant, dimensionless 

\( \gamma \), microlayer geometrical factor, dimensionless 

\( \delta \), microlayer thickness, [m] 

\( \Delta \), meaning ‘difference’ 

\( \varepsilon = \sqrt{\lambda \rho c} \), thermal effusivity \([s^{1/2}/m]\) 

\( \phi \), color function, dimensionless 

\( \lambda \), thermal conductivity \([W/m/K]\) 

\( \mu \), dynamic viscosity \([Pa\times s]\)
\( v \), bubble release frequency \([s^{-1}]\)

\( \psi \), rate of molecular collisions with a surface \([m^{-2}s^{-1}]\)

\( P \), thermal resistance \([m^2K/W]\)

\( \sigma \), surface tension coefficient \([N/m]\)

\( \tau \), bubble release period \([s]\)

\( \vartheta \), contact angle \([\text{degrees}]\)

\( \zeta \), artificial interface viscosity, \([m^2s^{-1}]\)

\( \Omega \), ratio evaporative/conductive thermal resistance, dimensionless

\( \nabla \), differential operator ‘nabla’, \([m^{-1}]\)

**Superscripts:**

· meaning ‘per unit time’

‘ meaning ‘per unit length’

” meaning ‘per unit area’

”” meaning ‘per unit volume’

- meaning ‘mean’

*, equilibrium value

’, meaning ‘dimensionless’

**Subscripts:**

\( \theta \), initial

\( \infty \), meaning ‘remote’

\( \text{avg} \), average

\( b \), bubble
bulk, referred to the bulk fluid

cell, of a cell

conv, convection

D, meaning ‘at lift-off’

dep, deposition

em, emission

ev, evaporation

F, fluid

gs, of the gas-solid interface

int, interface

l, liquid

ls, of the liquid-solid interface

lv, at the liquid-vapour interface

mech, mechanistic

min, minimum value

ml, microlayer

p, at constant pressure

ps, referred to pseudo-time

q, quench

qs, quasi-steady conduction

ref, reference value

s, solid

SAT, at saturation

site, of nucleation sites

sl, at the solid-liquid interface
\( \sigma \), surface tension

\( T \), thermal layer

\( th \), thermal

\( tc \), transient conduction

\( v \), vapour

\( w \), at the wall

\( wait \), wait time

**Non-dimensional quantities**

\[
Ja = \frac{\rho_c \mu (T - T_{SAT})}{\rho_v \mu_f \beta}, \quad \text{Jakob number}
\]

\[
Nu = \frac{h_l}{\lambda}, \quad \text{Nusselt number}
\]

\[
\bar{T} = \frac{T - T_{SAT}}{T_{w} - T_{SAT}}, \quad \text{dimensionless temperature}
\]

**List of acronyms**

BWR – Boiling Water Reactor

CFD – Computational Fluid Dynamics

CHF – Critical Heat Flux

CIP-CSL – Constrained Interpolation Profile with the Conservative Semi-Lagrangian scheme

DNB – Departure from Nucleate Boiling

DNS – Direct Numerical Simulation

ITM – Interface Tracking Methods

LS – Level-Set

LWR – Light Water Reactor

PSI-BOIL - Parallel Simulator of BOILing phenomena
PWR – Pressurised Water Reactor

RPI – Rensselaer Polytechnic Institute

VOF – Volume Of Fluid
CHAPTER 1

INTRODUCTION

This thesis describes a project on microscopic modelling of nucleate boiling phenomena. In this introductory chapter, the author gives context to the subject matter, with a brief discussion of the importance of boiling heat transfer in the context of water-cooled nuclear reactors. The scope, and main contributions, of the project are stated. An outline of this thesis is presented.

1.1 Background and motivation

The boiling process is of great importance to the design and operation of LWRs.

During normal operation of water-cooled reactors, liquid water is turned into steam in a controlled way. In PWR cores, a slight degree of subcooled nucleate boiling is maintained in order to enhance heat removal from the fuel rods, while in most of the heated length of BWR cores, vigorous boiling occurs, with much of the length actually undergoing boiling in the annular flow regime.

From the point of view of normal design, the importance of being able to predict CHF conditions, at which controlled boiling degenerates, causing an uncontrolled increase in clad temperature, and the fuel damage that follows, is obvious. A typical example is the characterization of conditions approaching ‘departure from nucleate boiling’ (DNB), and the recommendation of suitable safety margins to be respected in order to operate at a distance from DNB.

In fault conditions, such as during the reflood of voided cores following loss of coolant accidents, virtually all boiling modes can occur, including extreme forms of vaporization. These include explosive boiling during rewet of heated rods, or vaporization of droplets impinging on the as yet non-wetted clad surface.

During the first few decades of nuclear thermal-hydraulics research, the approach to modelling boiling flows was phenomenological in nature, and the vast majority of predictive tools were based on empiricism. Later on, more mechanistic techniques reached the level of
maturity required for reliable application to two-phase flow problems of relevance to the nuclear industry. These techniques, broadly within the framework of CFD, were based on a phase averaged, two-fluid approach, capable of useful predictions from an engineering point of view. By their own nature, these tools required closure relations accounting for the microscopic mechanisms that determine the wall-to-fluid and phase-to-phase mass, momentum and energy transfer. In particular, achieving reliable closure relations for wall-to-fluid energy transfer in boiling conditions posed delicate challenges. Attempts at undertaking these challenges pointed at the need of much detailed modelling work aimed at providing data and insights to improve the overall methodology.

These ‘macro-scale’ methods, relying on a priori assumptions about the flow regimes they were applied to, were not devised to give insight on the dynamics of two-phase flows at a fundamental level. To this end, the one-fluid formulation, capable of tracking the evolution in time of the gas-liquid interface, has been introduced recently by the CFD community. This family of Interface Tracking Methods (ITM) shows great promise, since they allow descriptions of the structure of multi-phase flows with unprecedented detail. In addition, they can be easily augmented to include mechanistic models of phase-change and chemical reactions.

The nuclear community has been receptive to this call for innovation in methodology, as demonstrated by several collective modelling efforts, and by local research projects, funded by major nuclear industrial partners. The ultimate motivation of these projects is to improve the efficiency and safety of nuclear systems, therefore limiting the cost and increasing the public acceptance of nuclear energy. With CHF being the main thermal-hydraulic constraint in the design of LWRs, investigations within the context of these international projects paid much attention to improving the understanding of boiling flows, with the future goal of predicting CHF mechanistically.

However, the state of the art is still far away from this goal (Yadigaroglu (2014)). At present, the modelling of isolated-bubbles boiling regimes, or even predicting the behaviour of a single nucleating bubble, pose a scientific challenge. Due to the local, transient nature of boiling, and its dependence on sub-processes occurring at very small lengths during short time scales, experimental techniques have been developed in
order to make detailed microscopic observation, with the aim of improving the current empirical understanding of boiling phenomena. In the same spirit, microscopic mechanistic modelling techniques, based on CFD with ITM, have in the last ten years or so begun to be applied to single-bubble growth problems, with the aim of improving semi-mechanistic representations of boiling flows at a larger scale, of industrial use, and of gaining better understanding of the boiling process itself.

1.2 Overview of nucleate boiling

During nucleate boiling, steam bubbles are generated from pre-existing vapour pockets at nucleation sites randomly distributed on the heated surface. Due to the large latent heat of water, the formation of a bubble provides a local heat sink, which partially accounts for the large cooling rates observed during boiling. Bubbles are also believed to act as ‘micro-pumps’, capable of pushing fluid at the remote temperature close to the surface, hence providing additional cooling. Furthermore, under certain conditions, a particularly efficient mode of heat removal from the surface is the evaporation of the thin liquid film, the microlayer, present beneath the bubble base.

The development of a complete understanding of nucleate boiling poses several challenges, the most pressing of which can be summarised by the following open questions:

- Does the bubble release process cause local enhanced liquid phase cooling of the boiling surface? Is it possible to quantify the associated cooling rates, and what is the relative importance of this heat removal mechanism?

- What is an adequate representation of the evaporation process at the liquid-vapour interface, suitable for incorporation in mechanistic modelling of bubble formation? Are different representations required to model evaporation at the bubble-curved surface and at the microlayer?

- What is the relative importance of evaporation from the bubble surface and from the microlayer as regards steam bubble formation?
For use within heat flux partitioning approaches to component-scale modelling, it is important to estimate accurately the different heat transfer mechanism, and the relative importance of each to the overall heat-removal performance. For example, the design of systems containing large populations of bubbles requires knowing the heat per bubble extracted from the heated surface by each sub-process. This is a typical issue in the development of ‘component-scale’ CFD models of boiling flows.

From a fundamental point of view, it is desirable to improve the understanding of the sub-processes themselves. For example, while the current phenomenological understanding of evaporation is adequate for standard design procedures, models conceived within extant theoretical frameworks have difficulties at explaining the most recent experimental findings.

1.3 Scope of the present work

The aim of this work was to develop analytical and computational models of the heat transfer and fluid flow associated with the formation and release of a single steam bubble during the boiling of water.

1.4 Contributions

1.4.1 Steam bubble growth rates

A new analytical method for predicting steam bubble formation due to evaporation at the bubble surface has been developed. Predictions so obtained are capable of favourable comparisons with experimental bubble growth at atmospheric and high pressure.

Fully resolved CFD computations of the hydrodynamics and heat transfer associated to steam bubble growth due to evaporation at the bubble surface have been developed, showing good agreement with analytical and experimental growth rates at atmospheric and high pressure.

1.4.2 Microlayer evaporation and the fundamentals of the vaporization process

The process of microlayer depletion due to evaporation has been analysed from a molecular point of view. Anomalies in recent reported experimental measurements have been explained
by the invoking of models of evaporation and condensation based upon kinetic theories. This analysis allowed the experimental measurements to be used to provide useful quantification of parameters that arise in this kinetic theory.

The analysis provided indications on the fundamentals of the evaporation process in general, but where these effects play a major role is microlayer evaporation. This improved understanding of the microlayer behaviour has been incorporated into the sub-model of an interface tracking code, and its effect explored.

1.4.3 Nucleate boiling heat transfer

The ‘quenching’ component is generally believed to be a major contributor to nucleate boiling heat transfer, and features via a very approximate model in such component scale boiling models. Detailed mechanistic modelling of the evaporation, bubble departure, and associated fluid flows, has permitted estimates to be obtained of the quenching heat transfer component via ‘first principles’. These have been compared to the estimates of quenching heat transfer generally incorporated in the flux partitioning treatments, and significant discrepancies have been identified.

1.5 Structure of the thesis

Short critical surveys of the relevant literature are presented at the beginning of each chapter, with the purpose of introducing the subject matter to be discussed. Comprehensive reviews are available in the works of Hewitt (1998), Dhir (1998), Kim (2009) and Dhir (2013).

The analysis of bubble-growth is the subject of Chapters 2, 3 and 4. In general, the bubble develops due to vapour generation at the curved surface and from its base, the latter due to evaporation of the microlayer. In the first part of the thesis, we consider cases in which the contribution of the microlayer is not important. This is typical of low (around unity or less) Jakob number conditions, which are characteristic of industrially relevant boiling situations, such as in a nuclear reactor. The models described in these initial chapters have been developed to predict bubble growth due to evaporation at the curved surface.

Chapter 2 describes a new method, based on an analytical energy balance applied at the bubble-curved surface, of predicting bubble growth at a heated substrate.
Chapter 3 describes the interface tracking methodology adopted in the CFD modelling presented in this thesis. The methodology is embodied in the code PSI-BOIL, which has been used in all the CFD simulations of this project.

In Chapter 4, CFD computations of steam bubble development, in isolation and at a surface, are discussed, and are compared with predictions from analytical modelling, and the effectiveness of the current capability is assessed.

In the following Chapters 5, 6 and 7, bubble growth, and the associated flows of heat and mass from the liquid and from the substrate, are considered in conditions in which microlayer evaporation is important. This is typical of Jakob numbers higher than ten. For the case of water and refrigerants, this mode of bubble growth has been mainly observed in laboratory conditions.

The Chapters 5 and 6 are devoted to the analysis of the fundamental evaporation process, and its application to studying microlayer depletion.

In Chapter 5, the thermal resistance, associated with the interphase matter transfer at the vapour-liquid interface, is discussed; its influence on steam bubble growth is assessed.

In Chapter 6, a model of microlayer evaporation based on a simple kinetic analysis is introduced, and evaluated in the context of resolving the inconsistency of a recent set of microlayer depletion measurements.

Chapter 7 describes the incorporation of this evaporative resistance in the microlayer sub-model of the PSI-BOIL code. An assessment of the effect of including evaporative resistance on modelled bubble growth is presented.

The hydrodynamics and heat transfer of a single bubble during pool boiling are the focus of the latter part of this thesis. This investigation has been conducted in order to elucidate the mechanisms of pool boiling heat transfer; in particular, to study the relative importance of the evaporation and transient conduction heat transfer components.

Transient conduction heat transfer following bubble release is the main subject of Chapter 8. This chapter presents an attempt to compute the ‘quench’ heat flux associated with the flow of liquid attendant upon the departure of a bubble from a heated surface. A mechanistic model of steam bubble formation is presented. The bubble growth process is followed by an
assessment of the heat transfer subsequent to its departure. This is compared to the heat transfer predicted by the simple ‘quench’ model in the heat flux partitioning treatment.

The thesis closes in Chapter 9 with a discussion of the main findings of this project. Recommendations for future work are suggested.
CHAPTER 2

THE PREDICTION OF BUBBLE GROWTH RATES:
ANALYTICAL APPROACH

The prediction of steam bubble growth rates is the subject matter of this chapter. A survey of extant physical models of bubble growth – both in isolation and at a heated wall – is presented. The main differences between the two cases, and how they have been addressed by analytical treatments, are discussed. The approach here proposed to model the wall-boiling case is introduced. An analytical model of a bubble growing at a heated surface due to evaporation at the bubble-curved surface is presented. The model accounts for non-uniform liquid superheat and departure of bubble shape from sphericity. Application of the model to nucleate boiling benchmarks is discussed.

2.1 Our current understanding of steam bubble development

In what is termed nucleate boiling, a vapour bubble nucleates at a solid wall from a pre-existing pocket of gas or vapour (a nucleation site) and grows as steam is generated. Two asymptotic regimes of expansion are possible. Very early bubble growth is essentially an isothermal process (Rayleigh (1917)), during which the factor limiting bubble growth rate is not the rate of production of vapour, but the rate at which momentum is transferred to the surrounding body of fluid (‘inertia-controlled bubble growth’). Subsequent bubble growth is limited by the transport of heat to the bubble surface (‘heat diffusion-controlled bubble growth’, Scriven (1958)), and that is the focus of this chapter.

When a vapour bubble grows on a superheated solid substrate, steam is generated via two complementary mechanisms, Figure 2-1.
Much of the steam is generated by evaporation from the curved surface, via relaxation of the temperature of the superheated liquid layer, of thickness $d_T$, surrounding the liquid–vapour interface.

Macroscopically, a time-varying slope of the bubble-curved surface is observed at the bubble base; the angle denoted as $\theta$ in Figure 2-1. However, the ‘contact’ between vapour and solid at the bubble base is only apparent: as the bubble grows, (under at least some conditions) a thin layer of liquid is observed to be left beneath it (Cooper and Lloyd (1969)). This liquid film is generally termed the ‘evaporation microlayer’, or simply ‘microlayer’. Being such a thin layer, the flow of heat through it is large, and presumably contributes significantly to bubble formation.

For the case of a bubble growing in water at atmospheric pressure, initiated at a rather typical wall temperature of 110 ºC, typical bubble lift-off sizes are 3-5 mm, typical superheated liquid layer thicknesses $d_T$ are approximately 0.4-0.7 mm, and typical microlayer thicknesses are approximately 1-5 micron.

2.2 Analytical models of steam bubble development

Early modelling efforts focussed on the growth of bubbles in isolation (away from solid boundaries), and will be reviewed first.

2.2.1 Physical model of a spherical bubble in an extensive pool of liquid

We follow here the development of Dergarabedian (1952), and assume that the pressure inside the bubble has decreased, after a short time (typically tens of microseconds) from

![Figure 2-1: Our current understanding of steam bubble development. Adapted from Carey (1992).](image-url)
inception, to the prevailing ambient pressure plus some contribution from the surface tension. In order to determine bubble expansion, liquid ablation is neglected, its importance being generally trivial, given the large difference in density for most liquid-vapour pairs. The vapour is considered to be at the saturation temperature $T_{\text{SAT}}$ at such pressure. At infinity, the liquid is at a constant temperature $T_{\infty}$, larger than saturation. The heat required to generate vapour and thus cause the bubble to grow is taken from a water layer surrounding its surface; the thermal boundary layer, or ‘relaxation layer’. The order of magnitude of its time-dependent thickness is approximately equal to $\sqrt{\alpha\delta t}$. For water at atmospheric pressure, the liquid thermal diffusivity $\alpha_l$ is of order $10^{-6} \text{ m}^2/\text{s}$, typical growth times are of hundredths of seconds and, using these numbers, an upper bound value of the thermal layer thickness is typically a few tens of microns, much smaller than typical bubble sizes.

![Figure 2-2: Physical model of spherical bubble growth in an extended pool of liquid.](image)

This will allow neglecting the effect of the spherical geometry of the system on the temperature distribution in the liquid.

The energy supplied by the thermal layer to the bubble between two close times $t_{i-1}$ and $t_i$, and consumed in growing the bubble from radius $R_{i-1} = R(t_{i-1})$ to radius $R_i = R(t_i)$ is

$$\frac{4}{3} \pi \rho \gamma h \left( R_i^3 - R_{i-1}^3 \right) \quad (2.1)$$
This corresponds to an amount of sensible heat, stored in the liquid, equal to

\[
\rho_l c_p \left( \sqrt{\alpha_l t_i} 4\pi R_{i}^2 - \sqrt{\alpha_l t_{i-1}} 4\pi R_{i-1}^2 \right) (T_\infty - T_{SAT})
\]

(2.2).

where the term in round brackets represents the volume (a spherical shell) of liquid in the thermal layer of thickness \(\sqrt{\alpha_l(t_i - t_{i-1})}\), and the reference temperature, above which the excess energy is computed, is the saturation value.

Equating these expressions of the latent and sensible heat:

\[
\frac{4}{3} \pi \rho_v h_g \left( R_{i}^3 - R_{i-1}^3 \right) = \rho_l c_p \left( \sqrt{\alpha_l t_i} 4\pi R_{i}^2 - \sqrt{\alpha_l t_{i-1}} 4\pi R_{i-1}^2 \right) (T_\infty - T_{SAT})
\]

(2.3)

If one takes \(R_{i} \approx R_{i-1}\), it is possible to write:

\[
\frac{4}{3} \pi \rho_v h_g \left( R_{i} - R_{i-1} \right) = \rho_l c_p \left( \sqrt{\alpha_l t_i} 4\pi - \sqrt{\alpha_l t_{i-1}} 4\pi \right) (T_\infty - T_{SAT})
\]

(2.4)

Making use of differentials, one gets the desired expression for the time-dependent bubble growth rate:

\[
\frac{dR}{dt} \approx 3\sqrt{\alpha_l} \frac{\rho_l c_p (T_\infty - T_{SAT})}{\rho_v h_g} \frac{d\sqrt{t}}{dt} = \frac{3\sqrt{\alpha_l} Ja}{2\sqrt{t}}
\]

(2.5),

where the Jakob number is defined as:

\[
Ja = \frac{\rho_l c_p (T_\infty - T_{SAT})}{\rho_v h_g}
\]

(2.6).

The Jakob number is the fundamental non-dimensional parameter determining bubble growth rates. Physically, it represents the ratio between the sensible heat stored in the liquid and the latent heat required to produce vapour. As such, it determines how vigorous is the evaporation causing bubble growth. To get a sense of scales, for the case of water at atmospheric pressure, and a superheat of 10 K, \(Ja = 30\); at the same superheat in BWR conditions (70 bar), \(Ja = 0.7\). In fact, much lower bubble-growth rates have been observed at high pressures (Labuntsov, Kol’chugin et al. (1964)) than at low pressures (Duan, Phillips et al. (2013)).
The time-dependent bubble radius can be expressed as:

\[ R(t) \simeq 3Ja\sqrt{\alpha_t t} \quad (2.7) \]

The time-dependent bubble radius is proportional to the thermal penetration depth in the liquid, via a non-dimensional group that contains the Jakob number and is usually referred to as a ‘growth constant’.

The simple models of Forster and Zuber (1954), Plesset and Zwick (1954) and Mikic, Rohsenow et al. (1970) are based on this physical understanding. For example, the popular growth constant computed by Plesset and Zwick is equal to \( \sqrt{\frac{k}{\pi}}a \).

A more complicated treatment is due to Scriven (1958), who solved the fundamental energy balance equation applied to an expanding bubble in spherical coordinates, under the assumption of spherical symmetry. The model thus accounts for the influence of the curvature of the bubble wall on the temperature distribution in the liquid.

Expressions for the time-dependent bubble radius and radial temperature profile in the liquid were found in the form of similarity solutions of the heat transfer problem. The bubble radius was found to increase with the square root of time with a growth constant \( \beta \), depending on fluid properties:

\[ R(t) = 2\beta\sqrt{\alpha_t t} \quad (2.8) \]

where the growth constant is obtained via numerical integration:

\[
\frac{\rho \lambda C_p \left( T_\infty - T_{\text{SAT}} \right)}{\rho_s \left( h_0 + \left( c_p - c_m \right) (T_\infty - T_{\text{SAT}}) \right)} = 2\beta^2 \int_0^\infty \exp \left\{ -\beta^2 \left[ \left( 1 - \xi^2 \right) - 2 \left( 1 - \frac{\rho_s}{\rho_l} \right) \xi - 1 \right] \right\} d\xi
\]

(2.9).

As a first approximation, if the thermal diffusivity of the liquid is small, then the thermal boundary layer is at all times small compared to the bubble radius, and the curvature of the liquid-vapour interface can be neglected. However, it can be shown from Scriven’s analysis
that the ratio between the thermal layer thickness and the bubble radius does not change during bubble growth, and that it decreases as the Jakob number increases. Growth constants obtained with or without including the effect of curvature are shown in Figure 2-3, where the model by Plesset and Zwick (which ignores the curvature) is compared to that of Scriven. At high Jakob numbers, no discrepancy is observed; however, at lower Jakob numbers, growth constants obtained neglecting the curvature of the system, and those obtained including it, are significantly different. At equal remote liquid temperature, the thermophysical properties of water are such that low (high) Jakob numbers correspond to high (low) pressures. The accurate treatment by Scriven is thus recommended when dealing with bubble growth in pressurised water.

![Graph](image)

Figure 2-3: Comparison of bubble-growth constants obtained with the treatment of Plesset (dashed line), and of Scriven (solid line).

### 2.2.2 Physical model of a bubble growing at a heated wall

The study of boiling for practical applications (power generation, cooling of electronic equipment) prompted the development of analytical tools to model bubble development in the presence of a heated substrate.
The two main differences between the wall-boiling case and the isolated bubble case are the non-uniform temperature distribution in which the bubble grows, and the presence of the microlayer beneath the bubble.

As regards computing evaporation at the bubble curved surface, the difficulty lies in including the variable superheat driving evaporation as the bubble grows, which is compounded if its cap grows beyond the superheated liquid layer.

Some authors, Han and Griffith (1965) and Mikic, Rohsenow et al. (1970), assumed that the whole of the bubble curved surface is enclosed in a relaxation layer of superheated liquid, pushed upwards by the bubble cap as the bubble expands, as shown in Figure 2-4.

![Figure 2-4: Physical model of a bubble enclosed in a superheated liquid layer, from Han and Griffith (1965).](image)

The nature of this hypothetical layer has been the subject of speculation, since no direct experimental observations of it have ever been made. According to Han and Griffith, its thickness is equal to that of the near-wall superheated layer $d_{T}$. Mikic proposed that this thickness is equal to a conduction layer that is formed during the wait time between the formation of two successive bubbles, essentially a thermal penetration depth in the liquid based on that time.

The heat-diffusion treatment developed for spherical bubbles in isolation was therefore augmented to take into account a non-uniform initial temperature distribution in the liquid by Han and Griffith (1965), or extended to include a geometrical factor accounting for the presence of the wall boundary, by Mikic, Rohsenow et al. (1970).
Other authors suggested that only the lower part of the bubble wall is surrounded by superheated liquid, as shown in Figure 2-5 for the extreme case of a bubble that is large compared to the near-wall superheated layer. In this case, evaporation occurs from only a fraction of the curved surface. This is the approach adopted by van Stralen, Sohal et al. (1975), who explicitly accounted for the height of the bubble compared to the superheated layer thickness.

![Figure 2-5: Physical model of a bubble expanding far beyond a superheated liquid layer, from Cooper (1969).](image)

As the thickness $d_T$ of the superheated liquid layer is significantly smaller than typical bubble sizes, this led to the conclusion that only a small fraction of the curved-surface is surrounded by superheated liquid, and therefore curved-surface evaporation is insignificant (Cooper (1969)).

More generally, a bubble is expected to be fully enclosed by superheated liquid during the early stages of growth; later on, a significant fraction of the bubble wall will inevitably be outside the superheated liquid layer, unless the superheated liquid layer is carried up by the bubble cap. Indeed, a detailed CFD investigation of this specific point would be interesting. Some investigation has been performed as part of the work for this thesis, but not sufficient for it to be formally included, although initial indications were that the layer was not carried up with the growing bubble.

The microlayer has been normally regarded as a stagnant, thin liquid film of negligible thermal capacity, its evaporation driven by the temperature difference between its lower (the solid-liquid interface) and upper (the liquid-vapour interface) surfaces (van Stralen, Sohal et al. (1975) and Cooper and Lloyd (1969)).
Taking the upper microlayer surface temperature as the saturation value at the prevailing ambient pressure is the usual approach. This value is usually significantly smaller than the temporally and spatially variable solid-liquid interface temperature, the extent of the discrepancy depending on the thermal properties of the substrate. Based on these assumptions, large temperature gradients across the microlayer are expected, and correspondingly large evaporation heat fluxes. This argument led to the conclusion that microlayer evaporation is the dominant mechanism of bubble formation, or at least that the vapour produced from evaporation of the microlayer was a significant amount of the overall production of vapour. This was presumed to be particularly the case when bubble formation is accompanied by small drops in temperature at the solid-liquid interface, a condition typical of high thermal conductivity substrates. We will return to the issue of proper modelling of the microlayer in the following chapters. In this present chapter, the effect of microlayer evaporation on bubble growth is neglected.

2.3 The bubble growth model here proposed

An improved methodology for predicting growth rates of bubbles forming at a heated surface is developed here. The model is based on an energy balance applied to the bubble-curved surface. The effect of non-uniform temperature distribution on bubble formation is included, under the assumption that evaporation occurs from only that fraction of the bubble surface that is within the superheated liquid layer, Figure 2-6. This effect is approximated introducing a Scriven-type growth constant computed based on the thickness of the superheated liquid layer, and on the temperature variation inside the layer. Since the elevation of the bubble cap varies with time, no closed relationship exists for the time dependent bubble radius, which is computed with a numerical procedure. The model also captures the departure from sphericity of the bubble shape, treating the curved surface as a truncated sphere. The extent of the departure from a full sphere is accounted for with the thermodynamic contact angle, which depends on the surface energies of the liquid-vapour, solid-liquid and solid-vapour interfaces.
Figure 2-6: Schematic of the proposed bubble-growth model.

The model is based on the following assumptions:

1. A layer of superheated liquid of uniform thickness $d_T$ exists above a heated wall at temperature $T_w$. Outside this thermal boundary layer the liquid is at the saturation temperature $T_{SAT}$ corresponding to the ambient pressure. Inside the boundary layer the liquid temperature falls linearly from $T_w$ to $T_{SAT}$.

2. Bubble growth occurs due to evaporation at the vapour-liquid interface.

3. The bubble retains the shape of a spherical cap with radius $R$ and contact angle $\theta$, which both vary with time.

4. The vapour inside the bubble is at a uniform temperature, the saturation temperature at the externally imposed pressure.

5. Spatial variations in the pressure inside the bubble, due to fluid dynamic and hydrostatic forces, are neglected.

Neglecting the presence of the microlayer is at the basis of assumption (3), which is predicated on the existence of a real contact line at the bubble base. This is likely to be the case at high pressures, and possibly at atmospheric pressure at moderate superheat (a few degrees). As such, this model is appropriate for these conditions.
2.3.1 Bubble growth rate

Under the above assumptions, energy conservation requires that the rate of change of bubble mass equals the flow of latent heat into the bubble. This can be expressed as:

\[ \rho_v \frac{dV_b}{dt} = S_b \overline{q''} \]

(2.10),

where the area-averaged heat flux at the curved-surface is

\[ \overline{q''} = \frac{1}{S_b} \int q''(z) dS_b \]

(2.11).

Using infinitesimal calculus it is possible to prove that for a sphere there is an equal amount of surface area in each elemental part of height \( dz \).

This fact is highly counterintuitive, but it will be explained with the help of the construction shown in Figure 2-7.

![Figure 2-7: Geometric construction used to show that for a sphere there is an equal amount of surface area in each elemental section of height \( dz \).](image)

It is required to show that the fraction \( dS_b \) of the surface of the sphere spanned by a rotation of the arc \( dl \) around the axis \( z \) does not depend on \( z \), i.e. it is the same if \( dl \) is taken at the equator or, say, halfway between the equator and one pole. The elemental area is

\[ dS_b = 2\pi a dl \]

(2.12).
The horizontal distance, $a$, from the $z$-axis of a point on the surface of the sphere can be expressed as a function of the radius, and of the latitude angle $\theta$:

$$a = R \cos \theta$$

(2.13).

An expression for $dl$ is now required. This arc will be approximated as a straight segment, since the height $dz$ is infinitesimal. The angle enclosed by $dl$ and $dz$ is equal to $\theta$. Then:

$$dl = \frac{dz}{\cos \theta}$$

(2.14).

Therefore the following expression is obtained for the elemental area:

$$dS_b = 2\pi R dz$$

(2.15),

which is independent of $z$. The surface of the sphere is obtained integrating this expression:

$$S_b = \int_{-R}^{R} dS_b = \int_{-R}^{R} 2\pi R dz = 4\pi R^2$$

(2.16).

Thanks to this result, it is possible to average the heat flux over the bubble elevation:

$$\bar{q''} = \frac{1}{z_b'} \int_{0}^{z_b'} \dot{q}''(z) dz$$

(2.17),

where $z_b(t)$ is the time-dependent bubble height.

The volume and surface area of the bubble depend on shape factors, which are functions of the contact angle:

$$V_b = \frac{4}{3} \pi R^3 g_1(\vartheta)$$

$$S_b = 4\pi R^2 g_2(\vartheta)$$

(2.18).

The heat flux into the bubble at a distance $z$ from the wall is assumed to be equal to that which would apply to a spherical bubble in isolation, growing in a uniform superheat equal to the actual superheat at this particular location $z$. In the problem here considered, this ‘virtual’ superheat $\Delta T(z)$ is a function of the distance $z$ from the wall, and is determined by the temperature variation in the superheated layer, known here by construction.
Let us now consider this virtual spherical bubble. The uniform, time-dependent heat flux into it can be expressed as

\[ \dot{q}'(t) = \rho v h g R(t) \]  
\[ \text{eqn. 2.19} \]

Calling the corresponding growth constant \( \beta(z) \), from Scriven’s solution the heat flux at a distance \( z \) from the wall can be written as

\[ \dot{q}''(z) = \rho v h g \beta(z) \frac{\alpha_t}{t} \]  
\[ \text{eqn. 2.20} \]

The space-dependent growth constant is taken to depend linearly on the local superheat \( \Delta T(z) \) at a distance \( z \) from the wall:

\[ \beta(z) = \frac{\beta_w \Delta T(z)}{\Delta T_w} \]  
\[ \text{eqn. 2.21} \]

where \( \beta_w \) is evaluated at the wall superheat \( \Delta T_w = T_w - T_{SAT} \) and the spatially variable \( \beta(z) \) is evaluated at the local superheat \( \Delta T(z) = T(z) - T_{SAT} \). In order to simplify the treatment, the bubble growth rate is expressed as function of the mean superheat over the curved surface \( \Delta T_b \):

\[ \dot{R}(t) = \beta_w \frac{\Delta T_b}{\Delta T_w} g_1(\vartheta) \frac{\alpha_t}{t} \]  
\[ \text{eqn. 2.22} \]

In order to compute \( \Delta T_b \), we recall that, inside the thermal boundary layer, the temperature decreases linearly with the vertical distance \( z \) from the wall, from a value \( T_{SAT} + \Delta T_w \) at \( z=0 \), to a value \( T_{SAT} \) at the distance \( d_T \):

\[ T(z) = T_w - (T_w - T_{SAT}) \frac{z}{d_T} \]

\[ \Delta T(z) = T(z) - T_{SAT} = (T_w - T_{SAT}) \left(1 - \frac{z}{d_T}\right) = \Delta T_w \left(1 - \frac{z}{d_T}\right) \]  
\[ \text{eqn. 2.23} \]

When the bubble is entirely within the superheated layer:
\[ \Delta T_b = \frac{1}{z_b} \int_0^{z_b} \Delta T(z) \, dz = \Delta T_w \left( 1 - \frac{z_b}{2d_r} \right) \]  

(2.24).

When the bubble tip protrudes outside the superheated layer:

\[ \Delta T_b = \frac{1}{z_b} \int_0^{z_b} \Delta T(z) \, dz = \Delta T_w \frac{d_r}{2z_b} \]

(2.25),

where the height of the bubble tip is a function of time \( z_b = z_b(t) \). Introducing a suitable Heaviside step function:

\[ H \left( \frac{d_r}{z_b} \right) = \begin{cases} 0 & \text{if } \frac{d_r}{z_b} < 1 \\ 1 & \text{if } \frac{d_r}{z_b} \geq 1 \end{cases} \]

(2.26),

it is possible to write a single expression for the mean liquid superheat:

\[ \Delta T_b = \Delta T_w \left[ H \left( 1 - \frac{z_b}{2d_r} \right) + \left( 1 - H \right) \frac{d_r}{2z_b} \right] \]

(2.27).

### 2.3.2 Bubble shape

By construction, the bubble retains the shape of a spherical cap with radius \( R \) and contact angle \( \vartheta \), which both vary with time. We here adopt a further simplification of assuming that dynamic effects associated to the rate of growth of the bubble do not change the contact angle. A constant contact angle, equal to the thermodynamic contact angle, is imposed:

\[ \vartheta = \vartheta' \]

(2.28).

The latter is defined by the Young-Laplace law as \( \text{Tryggvason, Scardovelli et al. (2011)} \)

\[ \vartheta' = \arccos \left( \frac{\sigma_{\nu} - \sigma}{\sigma} \right) \]

(2.29).

This simplification was justified \textit{a posteriori}, via comparison with mechanistic computations of bubble growth with the ITM, whereby the tangent angle is computed dynamically, which
gave results in good agreement with the present model. We will return to this point in the next chapter.

Rather than the surface energies, the contact angle itself is specified as an input, for a given fluid-surface combination.

In order to determine the truncation of the spherical bubble-curved surface, expressions are needed for the shape factors. These are available in standard geometry textbooks (Mathworks (1999)), and their derivation will not be shown here. The shape functions can be expressed as:

$$g_1 = 0.25\left(-\cos^3 \vartheta^* + 3\cos \vartheta^* + 2\right)$$
$$g_2 = 0.5\left(1 + \cos \vartheta^*\right)$$

The desired expression of the growth rate is then:

$$\hat{R}(t) = \beta \frac{g_2}{g_1} \frac{\Delta T_b(t)}{\Delta T_w} \sqrt{\frac{\alpha_w}{t}} = \beta \frac{2(1 + \cos \vartheta^*)}{\left(-\cos^3 \vartheta^* + 3\cos \vartheta^* + 2\right)} \frac{\Delta T_b(t)}{\Delta T_w} \sqrt{\frac{\alpha_w}{t}}$$

In principle, the time-dependent bubble radius could be found via integration of this expression. No close analytical expression was found for the time-dependent bubble radius. Therefore, (2.31) was integrated numerically by backward differencing, recalculating the value of $\Delta T_b$ at each time-step using equation (2.27).
2.4 Application of the model to pool boiling test cases

The analytical formulation described in the preceding text is applied to predict bubble growth in conditions broadly representing two sets of pool boiling measurements, those of Siegel and Keshock (1964) and those of Sakashita (2011). The input data are summarised in Table 2-1.

<table>
<thead>
<tr>
<th>Case</th>
<th>p [bar]</th>
<th>$\Delta T_w$ [K]</th>
<th>$d_T$ [mm]</th>
<th>Ja</th>
<th>$\theta^*$ [deg]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Siegel</td>
<td>1</td>
<td>6.17</td>
<td>0.742</td>
<td>18</td>
<td>40</td>
</tr>
<tr>
<td>Sakashita</td>
<td>45</td>
<td>1.83</td>
<td>0.932</td>
<td>0.18</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2-1: Input for the evaluation of the analytical model used to compute bubble growth due to evaporation at the curved surface.

2.4.1 Atmospheric pressure case

Figure 2-8 shows a comparison between analytical formulations of bubble growth that neglect the non-uniform temperature distribution near the wall (of Scriven and Plesset and Zwick), and the model here described constructed to include the effect. In the former case, the growth constant is the one that would apply to a uniform temperature body of liquid at the wall temperature. A large discrepancy is observed between the two approaches, especially at late times during bubble formation, when the bubble tip is well outside the superheated liquid. In passing, it is noticeable that in atmospheric conditions the error in computing the bubble size associated with neglecting the curvature of the bubble wall is negligible, as indicated by the small discrepancy between the Plesset and Zwick model (neglecting the curvature), and the Scriven model (including the curvature).
Good agreement between the present model and measured time history of bubble radius is observed, Figure 2-9. Since this good agreement is obtained without inclusion of microlayer evaporation in the analysis, it perhaps indicates that indeed microlayer evaporation is not significant under the conditions studied.
2.5 High pressure case

Growth curves from application of bubble-growth analytical models of Plesset and Zwick and Scriven to the high-pressure benchmark are shown in Figure 2-10. Both approaches model bubble growth in a uniform body of liquid at the wall temperature. If the Plesset and Zwick model is used, considerable error is associated with neglect of curvature of the spherically symmetric temperature distribution around the bubble.

Leaving Plesset and Zwick, we now compare the Scriven prediction with that of the present model, which does allow for a non-uniform temperature in the superheated liquid. We see that no significant change in prediction accompanies this modelling of the non-uniform temperature, due to the small size of the bubble compared to the thickness of the superheated layer, Figure 2-11.
Figure 2-10: Comparison of bubble-growth analytical formulations applied to high-pressure pool boiling conditions: effect of curvature.

Figure 2-11: Comparison of bubble-growth analytical formulations applied to high pressure pool boiling conditions: effect of non-uniform temperature distribution.

The time history of measured equivalent bubble diameter was compared against predictions of the analytical model, Figure 2-12. Good agreement is observed.
2.6 Concluding remarks

In this chapter, the development of a Scriven-type modified bubble-growth treatment has been described and tested. A presumed linear variation of the temperature difference driving bubble growth has been accommodated in the analysis. Simplifying assumptions, neglecting factors believed unimportant as regards bubble growth, were needed in order to come to a tractable model formulation. One important simplification is that the model is predicated on the assumption that bubble expansion is driven by evaporation at the curved surface; evaporation of the microlayer is neglected. Another simplification is related to modelling bubble shape, which is done via the imposition of a contact angle. The assumptions were justified \textit{a posteriori} by the good agreement with measured bubble growth for the model problems considered, but plainly they might not be justified in different conditions.
CHAPTER 3
INTERFACE TRACKING METHODOLOGY

The chapter begins with a condensed survey of Interface Tracking Methods for two-phase flows with phase change. An overview of the most significant developments in the field of ITM for boiling applications is presented. Crucial issues are identified, which point at the limitations of the approach, and indeed provide indications about the need of further developments in order to overcome such limitations. A description follows of the ITM here adopted, and of how it is coupled with a finite volume CFD representation of the fluid flow and heat transfer equations for incompressible flows, embodied in the code PSI-BOIL.

3.1 Background: the one-fluid model of two-phase flow

Interface tracking methods (Tryggvason, Scardovelli et al. (2011)) are CFD techniques whose aim is to simulate the temporal evolution of the interface between fluid phases. For the case of interest here of gas-liquid flows, typical examples of interfacial flows that can be modelled with ITMs are those resulting from an imposed velocity field, or by the action of gravity.

ITMs have been developed within the theoretical framework of the instantaneous formulation of the two-phase flow problem, which is mainly due to the work of Ishii (1975). At the basis of the approach, is the assumption that the interface can be described as a zero-thickness, massless surface. Among the various building blocks of the CFD methodology, the ITM is the component devoted to tracking the topological changes of the interface. In the most common approach, evolution of the flow field is described with one set of Navier-Stokes equations, allowing for variable fluid properties, their distribution a consequence of the distribution of phases captured by the ITM. Similarly, the discontinuities in macroscopic quantities, such as the pressure, occurring at the interface, are not explicitly enforced, which would require solving one set of transport equations per phase. Rather, they are incorporated into the one-fluid equations with local terms, present only in the immediate vicinity of the interface (Tanguy, Sagan et al. (2014)).

This approach is suitable for immiscible isothermal flows, and is fully mechanistic in the sense that its predictions are the result of solving the fundamental transport equations alone.
3.2 Extant CFD modelling of bubble growth

Non-isothermal flows of two phases of the same substance, such as vapour-liquid flows, require additional modelling. Firstly, an energy balance equation is required. Provided a suitable thermal specification of the interface (an issue which itself poses a delicate modelling challenge, as will be seen later), the approach would still be fully mechanistic, if capturing interphase mass transfer were not required. This does not follow from solution of the fundamental transport equations, and is the crucial issue for the application of ITMs to boiling flows. Additional modelling, outside the fluid flow formulation, is required to compute the local phase change in proximity of the interface (Tanguy, Sagan et al. (2014)).

At present, no comprehensive phase-change model exists that is capable of predicting the evolution of an embryonic vapour seed through all the stages of bubble growth. This is a consequence of the differences in physical processes involved in bubble behaviour.

For the particular case, of interest here, of bubble expansion, two different regimes of bubble behaviour can be isolated.

One is that of bubble dynamics (Brennen (1995)), and broadly it encompasses all situations in which the pressure in the interior of the bubble is different from the externally imposed pressure. This is typical of cavitation, or of the ‘inertial’ bubble growth.

For most bubble growth problems (Forster and Zuber (1954)), it is usually the case that the production of vapour at the interface is not vigorous enough to maintain the initial overpressure of the interior of the bubble. No equation of state is then explicitly required to link pressure and temperature inside the bubble, or at the interface. On the other hand, often is the case that it is required to predict the isobaric evolution of a bubble, as a consequence of the transport of sensible heat towards its surface. Indeed, the latter regime is relevant for the description of boiling flows in the context of the design of LWRs.

CFD analysis of bubble formation due to the addition of heat from the surrounding liquid was pioneered by the VOF-based method of Welch and Wilson (2000) and by the Level-Set method of Son, Dhir et al. (1999). More accurate analyses are due to the VOF method of Fuchs, Kern et al. (2006) and Kunkelmann and Stephan (2009). In these approaches, the boundary between the two incompressible phases is tracked with an advection-diffusion equation, as
with the popular LS and VOF methods. The thermal problem, whereby the vapour is normally taken at the saturation temperature at the prevailing pressure, requires modelling the evaporation at the curved surface. To this end, the flux of vapour into the bubble is computed from the energy balance applied to the vapour-liquid interface. It is most common to take the liquid-vapour interface to be at the equilibrium saturation temperature at the system ambient pressure. In a different approach (Hardt and Wondra (2008)), addressing largely refrigerants rather than water, some workers (Jia, Zhang et al. (2014)) have included deviations of the interface temperature from equilibrium. A more general treatment of the thermal boundary condition at the liquid-vapour interface is due to the Front Tracking technique of Juric and Tryggvason (1998), which was applied to film- rather than nucleate boiling.

More recently, a mechanistic, quantitative computational analysis of steam bubble development was developed by Sato and Ničeno (Sato and Ničeno (2013), Sato and Ničeno (2015)), who pioneered a physical model of bubble-curved surface evaporation capable of mesh convergent results. This evaporation model was applied to spherical bubbles and wall-boiling, and was similar in spirit to an earlier, Level-Set based treatment of Gibou, Chen et al. (2007). However, the authors noted difficulties in capturing bubble-curved surface evaporation rates, due to the thinness of the thermal boundary layers to be resolved by the computational grid (we recall the low value of the thermal diffusivity of liquid water), an issue addressed also by the analysis of Can and Prosperetti (2012). A different approach is that of Badillo (2012), based on a diffuse-interface description of the vapour-liquid interface, which accurately reproduced both experimental and analytical growth curves of spherical bubbles in isolation, if a fine discretization was used.

For practical purposes, the main conclusions of these analyses relate to the discretization needed to capture temperature gradients in the liquid at the bubble wall, based on which the evaporation rate is computed. As a rule of thumb, it can be concluded that in order to obtain accurate results, no fewer than three mesh points are needed in the relaxation layer. For most fluids of interest the temperature gradient exists over a distance, which is small compared to the bubble radius, as discussed. This fact limits the applicability of these techniques to industrially relevant problems. The ensuing need of large computational power, or of adaptive mesh refinement, has been discussed in Dhir (2013).
3.2.1 The issue of the thermal specification of the interface

The works summarised in the preceding text were all based on a simplifying assumption regarding the thermal specification of the interface, which was taken at the saturation temperature at the system pressure. This assumption is required in order to reduce the complexity of evaluating the energy balance at the interface. The notable exceptions were the work of Can et al., who applied the ideal gas law to the vapour in the interior of the bubble, and the work of Juric et al., where a rigorous thermal characterization of the interface was derived. In the latter work, the interface temperature depended non-linearly on a combination of evaporation rate, surface tension, difference in specific heat between vapour and liquid, and also resistance to interphase mass transfer, the latter not unlike the work of Hardt et al. and Jia et al., which are considered as special cases.

Deviations of interface temperature from saturation due to resistance to mass transfer and surface tension effects can be in principle important, depending on operating conditions, fluid properties, size of the system. The former effect is important only for the case of very small bubbles (radius of microns or below), and can be disregarded since in this work much larger systems are considered. The latter effect will be addressed in Chapter 5.

3.3 The CFD methodology here adopted

Use is made of the CFD methodology embodied in the code PSI-BOIL. The interested reader will find details in the following publications: Sato and Ničeno (2012), Sato and Ničeno (2012), Sato and Ničeno (2013), Sato and Ničeno (2015). Here a condensed description is presented.

3.3.1 Interface tracking

The incompressible Navier-Stokes equations, discretized according to the Finite Volume method, are solved, for the case of variable fluid properties, with a projection method, under the assumption of laminar flow. Mechanical properties are assumed constant, and uniform within each phase. The interface is located with the colour function approach, whereby the evolution in time of the liquid volume fraction distribution is computed with an advection diffusion equation. The CIP-CSL method of Takewaki and Yabe (1987) is used to advect the spatial distribution of the liquid volume fraction. The solution procedure consists in an advection step, taking into account injection of vapour into the bubble due to evaporation at
the vapour-liquid interface, and in a ‘sharpening’ step, required in order to prevent numerical
distortion of the interface.

Computation of a signed distance function from the colour function distribution follows the
sharpening step. Such a distance function is needed to compute the curvature of the vapour-
liquid interface, used to evaluate the surface tension and wall-adhesion terms of the Navier-
Stokes equations. These are treated as body forces according to the CSF method of Brackbill,
Kothe et al. (1992). The complete set of equations describing the hydrodynamic problem is as
follows:

\[
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \left( \nabla \cdot (\mathbf{uu}) - \mathbf{u} (\nabla \cdot \mathbf{u}) \right) = -\nabla p + \nabla \cdot \left( \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right) + \mathbf{f} \tag{3.1}
\]

(momentum balance)

\[
\nabla \cdot \mathbf{u} = \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right) \dot{m}^m \tag{3.2}
\]

(continuity)

\[
\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \mathbf{u}) = -\frac{\dot{m}^m}{\rho_l} \tag{3.3}
\]

(colour function advection).

In the equations above, a generic fluid property \( a \) depends on the color function \( \phi \) according
to the following expression:

\[
a = a_l \phi + a_v \left( 1 - \phi \right) \tag{3.4}
\]

where the subscripts \( l \) and \( v \) denote, respectively, the liquid and vapour phases. The color
function physically represents the volume fraction of liquid, and it assumes the value of 1 in
the liquid and of 0 in the gas.

Sharpening of the color function distribution is obtained integrating in pseudo-time to
steady-state the following equation (Olsson and Kreiss (2005)):
\[ \frac{\partial \phi}{\partial t_p} + \nabla \cdot \left( \phi (1 - \phi) n \right) = 0 \]  

(3.5).

Adding a viscous term to the right hand side of this equation was found necessary by Olsson et al., in order to avoid a discontinuity of the color function at the interface:

\[ \frac{\partial \phi}{\partial t_p} + \nabla \cdot \left( \phi (1 - \phi) n \right) = \zeta \nabla \cdot \nabla \phi \]  

(3.6).

This was found by Olsson et al. to enforce a constant interface thickness, proportional to \( \zeta \).

In the variant of the CIP-CSL method here adopted (Sato and Ničeno (2012)), an additional local parameter \( \eta \) is introduced, in order to perform the sharpening only in the regions of the interface that become the most distorted:

\[ \frac{\partial \phi}{\partial t_p} + \eta \nabla \cdot \left( \phi (1 - \phi) n \right) = \eta \zeta \nabla \cdot \nabla \phi \]  

(3.7).

The parameter \( \eta \) varies according to the flow details, taking values between zero and one. The largest the \( \eta \)-value, the largest the local correction of the interface thickness.

Following the sharpening procedure, the color function is converted into a signed distance function, with the method of Russo and Smereka (2000).

The surface tension force is computed based on the local curvature, assuming a constant surface tension coefficient, and on the color function:

\[ f_\sigma = \sigma \kappa \nabla \phi \]  

(3.8).

The gradient of the color function is non-zero only in proximity of the interface, which preserves the local nature of the surface tensions force. However, in the discrete approximation, it will inevitably be smeared on a few cells around the interface.

The curvature is computed from

\[ \kappa = - \left( \nabla \cdot n \right) \]  

(3.9).
Away from wall boundaries, the unit normal to the interface is computed based on the signed distance function as

$$\mathbf{n} = \frac{\nabla F}{|\nabla F|} \quad (3.10).$$

At wall boundaries, computation of the interface normal needs to be modified in order to accommodate the wall-adhesion force. The unit vector normal to the interface depends on the input equilibrium contact angle $\vartheta^*$ and on the wall-normal and wall-tangent vectors, according to the schematic of Figure 3-1.

![Figure 3-1: Definition of the unit normal vectors used in computing the wall adhesion force.](image)

In the layer of cells adjacent to the wall boundary, the unit normal to the interface is computed as follows:

$$\mathbf{n} = \mathbf{n}_w \cos \vartheta^* + \mathbf{n}_t \sin \vartheta^* \quad (3.11).$$

The actual tangent angle $\vartheta$, representing the slope of the liquid-vapour interface at the solid wall, varies in time according the balance of forces on the interface.

### 3.3.2 Heat transfer and phase change

Heating of the fluid due to compressibility and viscous effects is neglected, and the variable-properties energy advection-diffusion equation is solved both in the liquid and vapour...
phases. Thermophysical properties are assumed constant, and uniform within each phase. The thermal problem is described by the following energy balance equation:

\[ c_p \left( \frac{\partial T}{\partial t} + \nabla \cdot T \mathbf{u} - T \nabla \cdot \mathbf{u} \right) = \nabla \cdot (\lambda \nabla T) \] (3.12).

Evaporation at the bubble surface is computed mechanistically from the energy balance at the vapour-liquid interface.

At the moderate (< 0.1 kg/m²s) interphase mass fluxes here considered, and in systems that are large in terms of thermal capillary lengths (Badillo (2012)), it is appropriate to use a formulation of the interfacial energy balance known as the ‘Stefan condition’ (Alexiades and Solomon (1993)). With this model, the interphase mass flux is evaluated as proportional to the jump in heat flux across the interface, Figure 3-2.

![Figure 3-2: Energy balance at the evaporating vapour-liquid interface used in the mechanistic computation of evaporation rates in ITM simulations. Adapted from Sato and Ničeno (2013).](image)

In this work, it is assumed that, when not in contact with heated walls, the vapour is at the equilibrium saturation temperature corresponding to the externally imposed system ambient pressure: the effect of the Laplace pressure on the equilibrium saturation temperature of the vapour is neglected here. Also the interface temperature is assumed equal to the saturation
value at the system ambient pressure, and the curvature correction of the interface temperature is neglected, as are non-equilibrium effects.

If there is direct contact between the vapour phase and heated walls (such as at the dry patch beneath a growing bubble), the vapour can be superheated, but the corresponding change in vapour pressure is not accounted for.

Under these assumptions, evaporation at the bubble wall is computed according to the following expression:

\[ \dot{m}_{\text{mech}} = \frac{q_l \cdot n - q_v \cdot n}{h_f} \cdot \frac{S_{\text{ad}}}{V_{\text{cell}}} \]  \hspace{1cm} (3.13)

The heat fluxes \( q = q \cdot n \) in the direction normal to the interface appearing in this expression are computed as the local normal temperature gradient, \( \frac{\partial T}{\partial n} \), respectively on the liquid (subscript l) and vapour (subscript v) sides of the interface. They are evaluated only in cells containing the interface, or in those immediately adjacent. These cells are called ‘interface cells’. The source terms accounting for evaporation in the continuity and color function advection equation are also non-zero only in the interface cells.

### 3.4 Micro-region model

#### 3.4.1 Need of micro-region models in CFD modelling of bubble growth

As the application of DNS techniques is increasingly gaining popularity, the need of addressing multiscale issues in the modelling of multiphase flows has became apparent (Tryggvason, Thomas et al. (2010)). This is especially the case for wall-boiling flows, since the interaction of a growing steam bubble with a heated substrate depends on processes at submicrometric length scales, which are small if compared to typical bubble sizes. This poses a challenge for mechanistic CFD computations of steam bubble formation, due the prohibitive discretization that would be required to resolve all the relevant scales.

Thanks to experiments and theoretical developments, the current understanding of the bubble-substrate interaction has produced simple semi-mechanistic representations that can be used to inform the CFD simulation. Following this approach, there is no need of resolving all the details of the bubble base region with a computational grid.
These representations are usually called micro-region models, to stress the fact they are off-line, algebraic computations that complement the heat transfer and fluid flow problem solved via proper DNS.

Micro-region models are classified as ‘microlayer models’ and ‘contact line models’, depending on the physical mechanism that they describe, and which is supposed to be active at the base of the bubble, as shown in Figure 3-3.

![Figure 3-3: micro-region models for bubble growth analysis. From Fischer, Gambaryan-Roisman et al. (2015).](image)

3.4.2 Extant micro-region models: contact line models

When the liquid-vapour interface is close (a few nanometres apart) to a solid substrate, the effect of inter-molecular forces, active between the liquid-vapour and solid-liquid interfaces, becomes important (Tryggvason, Scardovelli et al. (2011)). Within certain fluids, inter-molecular forces cause a so-called ‘disjoining pressure’ at the liquid-vapour interface, of magnitude up to tens of kilopascals (Wayner, Kao et al. (1976)). At the bubble base, the liquid-vapour interface reaches very close to the wall, to form an apparent contact line. It is believed by some authors that a disjoining pressure arises there, and is present during all stages of bubble growth.

Contact line evaporation models are based on the hypothesis that the disjoining pressure can alter the evaporation mechanism, promoting vigorous net vaporization in the very narrow region around the apparent contact line. It is believed that the magnitude of the vapour production at the contact line is close to the kinetic limit (Maroo and Chung (2013)). While the
mechanism is not fully understood, several authors proposed models aimed at quantifying the evaporation rate around the disjoining-pressure affected region, the so-called ‘contact line evaporation models’. The contact-line physical model, and an indicative peak in heat flux that it predicts, are sketched Figure 3-4. These kind of treatments, such as that of Stephan and Busse (1992), have been used in CFD simulations of steam bubbles (Kunkelmann (2011)) in order to compute the contact line contribution to vapour generation, which can in principle be important (if not dominant) as regards bubble formation. This physical understanding of the contact line is not supported by direct experimental observations of the temperature and heat flux distribution at the solid surface beneath the bubble, such as those of Golobic, Petkovsek et al. (2007) or Jung and Kim (2014). These detailed microscopic measurements did not provide evidence of contact line enhanced evaporation. On the other hand, they showed a much smaller heat flow over a larger fraction of the bubble base area (Jung and Kim (2014)). This has been demonstrated to be the consequence of the evaporation of the microlayer, the thin liquid film occupying much of the bubble base, Figure 3-5. Contact-line models can effectively be considered superseded by these observations.

Figure 3-4: contact line evaporation models. From Wang, Garimella et al. (2008).

CFD simulations are thus required to include a means to compute evaporation from the extended thin film, not from the contact line, in order to produce adequate estimates of steam bubble development.
3.4.3 Extant micro-region models: microlayer models

The analysis of microlayer depletion due to evaporation, and the related flow of heat from the substrate to the liquid film, was first developed by Cooper (1969), who modelled the heat transfer through the layer as quasi-steady conduction, driven by the temperature difference between the upper and lower surface of the film. Guion et al. coupled the analysis to a mechanistic computation of bubble growth at a constant temperature surface (Guion, Langewisch et al. (2013)). Sato and Ničeno (2015) developed a ‘depletable’ microlayer model, accounting for the reduction in thickness of the film and increase in radius of the dry patch due to film evaporation, which included conjugate heat transfer with the solid. These models were prompted by experimental observations of the liquid film, and relied on empirical parameters (Utaka, Kashiwabara et al. (2013), Utaka, Kashiwabara et al. (2014)), such as the initial thickness of the film, in order to represent its behaviour. This constitutes a major difference with the previous generation of models, the contact-line models, which were based on theoretical developments.

![Microlayer evaporation models](http://example.com/microlayer_models)

Figure 3-5: microlayer evaporation models. From Guion, Langewisch et al. (2013).

3.5 Depletable microlayer model

We follow here the development of Sato et al.

To ‘start’ the CFD computation, a seed of vapour, of radius equal to one cell of the CFD mesh, is placed in the CFD domain at the nucleation site chosen. (This eventually grows to form the
bubble; given the small size of the initial seed, the influence of its initial shape or size on bubble growth is negligible.)

As vapour is generated, the volume of this bubble increases, by growing both upwards and radially outwards. So far as the CFD is concerned, this radial outwards movement of the interface is associated with the generation of a circular ‘dry’ surface beneath the bubble.

However, this radial growth is accompanied by the ‘leaving behind’ of a thin layer of liquid. It is in the sub-grid microlayer model that the formation and evaporation of this microlayer are taken into account.

The initial microlayer variation of thickness in the radial direction is a free parameter. It is normally modelled as being proportional, via a constant that we term $C$, to a chosen power $\gamma$ of the radial distance from the nucleation site. With $\delta$ the microlayer thickness, and $r$ the distance from the nucleation site, $C$ and $\gamma$ are the free parameters.

$$\delta_0(r) = Cr^\gamma$$ (3.14)

The subscript ‘0’ on the microlayer thickness is to distinguish its initial value; this thickness is then depleted as evaporation takes place.

In Figure 3-6 is shown such typical microlayer model geometry, here shown some little way into the computation.

Flow of liquid in the microlayer is neglected, as is the sensible enthalpy flow to the vapour. The microlayer thermal model is based on the hypothesis that the liquid film is thermally thin relative to the boiling substrate. It models heat transfer through the film as quasi-steady conduction in the vertical direction $z$ only; see Figure 3-6. By construction, the upper surface of the microlayer is at the saturation temperature at the system ambient pressure. The local transient heat flux is then:

$$\dot{q}^{\nu}_{mi} = \frac{T_d - T_{sat}}{\delta} \lambda$$ (3.15)

where the solid-liquid interface temperature and microlayer thickness values are understood to be temporally and spatially (along $r$) variable.
During bubble growth, the outer radius of the microlayer is the bubble base radius, the variation with time of which is computed by the interface tracking method within the normal CFD treatment.

The inner edge location (the ‘dry patch’ radius) is computed via the thermal coupling between the microlayer model and conduction in the solid substrate. The resulting radially varying heat flux normal to the solid-liquid interface is converted to an (also radially-varying) evaporative mass flux. This mass flux is allowed to deplete the thickness of the microlayer at that radial location:

$$\frac{d\delta}{dt} = -\frac{1}{\rho_v h_{ls}} \frac{\dot{q}''}{\dot{m}}$$ (3.16).
When this thickness goes to zero the microlayer model locally is ‘turned off’, and the dry patch centred on the nucleation site is thereby taken to have increased in radius.
CHAPTER 4
COMPUTATIONAL ANALYSIS OF STEAM BUBBLE DEVELOPMENT

This chapter describes a computational study of steam bubble formation as a result of evaporation at the bubble-curved surface. Predictions of bubble growth rates obtained with ITM simulations and with the analytical model introduced in Chapter 2 are presented. Comparisons between steam bubble growth rates, from the ITM and from analytical modelling, are shown at atmospheric and higher pressures. For the atmospheric pressure case, a pool boiling benchmark is considered. For the high-pressure case, bubble growth in isolation is considered first. The analysis is then extended to the wall-boiling case. In the analytical and CFD modelling of the wall-boiling cases, the effect of microlayer evaporation is not accounted for. Analytical growth rates and predictions of ITM agree well, despite the occurrence of spurious currents generated by the ITM at higher pressures. Remedies to prevent the spurious currents from arising are discussed.

4.1 Atmospheric pressure benchmark: the Siegel and Keshock experiment

4.1.1 Experimental arrangements by Siegel and Keshock

In the experimental arrangements devised by Siegel and Keshock (1964), the working fluid was water at atmospheric pressure, boiling in Earth gravity on an upward facing horizontal surface, Figure 4-1. Bubbles were observed at distinct nucleation sites on the surface. For comparison with results of CFD analysis, use is made of photographic evidence of bubble development at a nucleation site where bubbles are initiated at 106.17 °C. This level of superheat corresponds to a Jakob number of approximately 18. Being the boiling substrate a thick slab of copper, a material with high (~ 400 W/m/K) thermal conductivity, a negligible drop in temperature at the solid-fluid interface was observed at bubble formation. For present purposes, sufficient evidence of a quasi-isothermal boiling substrate was deduced from the investigation of Siegel and Keshock, which allowed ignoring the thermal response of the solid in the computational model.
Figure 4-1: Experimental arrangements by Siegel and Keshock (left), observations of steam bubble development (right). Adapted from Siegel and Keshock (1964).

4.1.2 Physical model of steam bubble development

The physical domain consists of a semi-infinite pool of liquid, bounded at its bottom by an isothermal no-slip surface, as shown in Figure 4-2. A constant value of the temperature, equal to the incipient nucleation temperature, is imposed at the solid boundary. A thermodynamic contact angle equal to 40° is imposed. This is the input value required by the CSF method. The tangent angle at the solid-liquid-vapour interface is dynamically updated as a consequence of the local flow details.
Figure 4-2: Physical model of steam bubble development used for ITM simulations of bubble-growth due to evaporation at the bubble-curved surface.

Ideally, the physical domain is not bounded, except at the aforementioned solid wall. In practice, a finite volume of liquid is simulated, bounded by fictitious walls.

During bubble growth, the details of the flow close to the fictitious boundaries of the domain are unknown a priori. Influence of boundary effects of the walls of the physical domain has been minimised choosing the largest size of the domain that yielded a size-independent bubble-growth curve.

4.1.3 CFD model

Circular symmetry of the bubble shape is assumed, allowing simulating only one quadrant of the physical domain. Dimensions of the computational domain, where the three dimensional unsteady transport equations, described in Chapter 3, are solved, are shown in Figure 4-3. Symmetry conditions are imposed at the x=0 and y=0 planes. Flow of heat and mass is not allowed across the remaining vertical boundaries. Flow of mass is allowed across the top boundary, where the saturation temperature (100 °C) is imposed. The thermophysical properties of water at 1 bar used in the analysis are summarised in Table 4-1.
As an initial condition, a vapour seed of radius equal to 1.5 times the cell size is placed at the bottom wall at the intersection of two vertical symmetry planes. The initial temperature distribution in the liquid decreases linearly with the vertical distance from the bottom surface. The drop occurs over a thickness of 0.742 mm, computed according to the correlation by Kays and Crawford (1993) for natural circulation on a horizontal surface. Outside the superheated layer, the liquid is initially at 100°C.

<table>
<thead>
<tr>
<th>Property</th>
<th>Water at 1 bar (Liquid)</th>
<th>Water at 1 bar (Vapour)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ [kg/m$^3$]</td>
<td>958.4</td>
<td>0.597</td>
</tr>
<tr>
<td>$\mu$ [Pa⋅s]</td>
<td>280.0x10$^{-6}$</td>
<td>12.5x10$^{-6}$</td>
</tr>
<tr>
<td>$\lambda$ [W/(m⋅K)]</td>
<td>679.0x10$^{-3}$</td>
<td>25.0x10$^{-3}$</td>
</tr>
<tr>
<td>$c_p$ [J/(kg⋅K)]</td>
<td>4215.9</td>
<td>2030.0</td>
</tr>
<tr>
<td>$\sigma$ [N/m]</td>
<td>59.0x10$^{-3}$</td>
<td></td>
</tr>
<tr>
<td>$h_{fg}$ [J/kg]</td>
<td>2258.0x10$^3$</td>
<td></td>
</tr>
<tr>
<td>$T_{sat}$ [K]</td>
<td>373.15</td>
<td></td>
</tr>
</tbody>
</table>

Table 4-1: Mechanical and thermophysical properties of water at 1 bar.

The initial vapour seed grows due to evaporation at the bubble-curved surface. Evaporation of the microlayer at the bubble based is here ignored, as is in all computations shown in this chapter.

The mechanistic computation of evaporation rates at the bubble wall embodied in the numerical method used here has been shown to depend on the discretization by Sato and Ničeno (2013). We recall that the evaporation rate is computed based on the normal heat flux
jump at the bubble wall (or equivalently, on the normal temperature gradient). In practice, it has been observed that the accuracy of such a computation depends on how finely the temperature distribution in the liquid adjacent to the bubble wall is discretized. A mesh convergence study was therefore conducted, its results summarised in Figure 4-4 and Figure 4-5. The levels of discretization used are summarised in Table 4-2.

<table>
<thead>
<tr>
<th>Mesh n.</th>
<th>Refinement index</th>
<th>$\Delta x_{\text{min}}$ [(\mu m)]</th>
<th>NXxNYxNZ</th>
<th>n. cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>44.8</td>
<td>33x33x52</td>
<td>56,628</td>
</tr>
<tr>
<td>2</td>
<td>0.5</td>
<td>22.4</td>
<td>66x66x100</td>
<td>435,600</td>
</tr>
<tr>
<td>3</td>
<td>0.25</td>
<td>11.2</td>
<td>132x132x200</td>
<td>3,484,800</td>
</tr>
<tr>
<td>4</td>
<td>0.125</td>
<td>5.6</td>
<td>264x264x380</td>
<td>26,484,480</td>
</tr>
</tbody>
</table>

Table 4-2: Discretization levels used in the mesh refinement study for the Siegel and Keshock low pressure bubble-growth benchmark.

![Figure 4-4: Mesh refinement study of the Siegel and Keshock low pressure bubble-growth benchmark: bubble growth curves.](image)
Figure 4-5: Mesh refinement study of the Siegel and Keshock benchmark: bubble sizes after 20 ms for various levels of discretization.

Based on available computational resources, cubic cells of side equal to 5.6 microns were used to discretize the region where the bubble develops. A total of 26,484,480 cells correspond to the discretization adopted. A plot showing a comparison between the time-dependent thermal penetration depth in the liquid $\delta_{th}$, and the fixed mesh size $\Delta x$ is shown in Figure 4-6.
4.1.4 Results of CFD analysis

The temperature distribution around the growing bubble is shown in Figure 4-7 at several times. The observed evolution of the bubble shape is a consequence of the initial superheated layer thickness and of the input thermodynamic contact angle. Both quantities are highly uncertain in conditions of interest, due to lack of experimental data. Different values of either would have resulted in a different evolution of the bubble shape.
Despite these uncertainties, qualitative remarks about the details of steam bubble formation are still possible thanks to CFD analysis. During the early stages, the bubble is fully within the superheated layer, as it was originally believed by Han and Griffith (1965) and Mikic, Rohsenow et al. (1970). The superheated liquid layer is actually pushed upwards by the bubble cap. Later on in the growth process, the vast majority of bubble-wall surface is out of the superheated liquid layer, and therefore surrounded by liquid at saturation, with no excess energy to drive further evaporation, as deduced by Cooper (1969).
At equal input thermodynamic contact angle (40°) and initial superheated liquid layer thickness (0.742 mm), the comparison between CFD modelling and the analytical model described in Chapter 2 is excellent, as shown Figure 4-8.

Figure 4-8: Comparison between bubble-growth analytical formulation and ITM analysis applied to atmospheric pool boiling conditions (Siegel and Keshock bubble-growth benchmark).

4.1.5 Comparison between CFD-modelled and measured bubble growth rates

Experimental growth curves obtained for four different bubbles growing at the same site and at the same inception superheat are compared against predictions of the CFD analysis and of the analytical model.
Figure 4-9: Comparison between modelled (analytical and with ITM) bubble radius as a function of time with experimental data collected by Siegel and Keshock.

The two modelled growth curves are in good agreement with experimental data. However, some aspects of the comparison will need further investigation. Firstly, the thermodynamic contact angle in boiling conditions is not available for the case at issue. The adopted contact angle is only a likely value, taken from the broad range typical of the so-called *partially wetting regime* (between 0 and 90 degrees), believed to be typical of most metallic surfaces. Secondly, the initial temperature distribution near the wall used to model bubble growth is taken from a correlation, and has not been validated due to lack of experimental data on the temperature distribution near the wall in conditions of interest.

In fact, the growth rate is sensitive to thermodynamic contact angle and superheated layer thickness. An increase of either quantity might cause an increase in the bubble growth rate. It is understood that similar agreement between computation and measurement could have been obtained with a smaller input contact angle and a thicker initial thermal boundary layer (or, vice versa, with a larger contact angle and thinner boundary layer). Perhaps more weight should be given to the comparison between CFD and analytical models than between modelled and measured growth rates.
4.2 Simulation of spherical bubble growing in a pool of pressurised liquid

The growth of bubbles in pressurised water is considered here. The case of spherical bubbles in isolation is analysed first, followed by a wall-boiling case.

4.2.1 Computational model

The simulation setup and material properties are shown respectively in Figure 4-10 and Table 4-3.

![Computational domain](image)

Figure 4-10: Computational domain to simulate the growth of a spherical bubble in isolation.

The conditions simulated are chosen to be broadly similar to published nucleate boiling experiments at high pressure conducted in normal (Earth) gravity, those of Sakashita (2011). The spherical symmetry of the problem is exploited to simulate a sector corresponding to only 1/8 of the physical domain; one quarter of the ‘top half’ of a bubble. The computational domain is a cube of side LX, with symmetric boundary conditions at the boundaries crossed by the gas-liquid interface and outlet conditions elsewhere. The normal pressure and temperature gradients are set to zero at the outlet boundaries. The domain size has to be chosen to accommodate the bubble and minimise the disturbance due to the outlet condition,
albeit constrained by computational cost. Geometrical and physical parameters for the two cases of interest are reported in Table 4-4. Initial conditions need to be specified. Inside the bubble, the vapor is set to the saturation temperature $T_{\text{sat}}$.

<table>
<thead>
<tr>
<th>Property</th>
<th>Water at 22.7 bar Liquid</th>
<th>Water at 22.7 bar Vapour</th>
<th>Water at 45 bar Liquid</th>
<th>Water at 45 bar Vapour</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ [kg/m$^3$]</td>
<td>830.0</td>
<td>13.5</td>
<td>787.6</td>
<td>22.7</td>
</tr>
<tr>
<td>$\mu$ [Pa·s]</td>
<td>117.3x10$^{-6}$</td>
<td>16.6x10$^{-6}$</td>
<td>103.0x10$^{-6}$</td>
<td>17.7x10$^{-6}$</td>
</tr>
<tr>
<td>$\lambda$ [W/(m·K)]</td>
<td>641.0x10$^{-3}$</td>
<td>45.2x10$^{-3}$</td>
<td>608.0x10$^{-3}$</td>
<td>53.7x10$^{-3}$</td>
</tr>
<tr>
<td>$c_p$ [J/(kg·K)]</td>
<td>4667.6</td>
<td>3486.3</td>
<td>4940.0</td>
<td>4230.0</td>
</tr>
<tr>
<td>$\sigma$ [N/m]</td>
<td>31.2x10$^{-3}$</td>
<td></td>
<td>24.5x10$^{-3}$</td>
<td></td>
</tr>
<tr>
<td>$h_{\text{fg}}$ [J/kg]</td>
<td>1821.5x10$^3$</td>
<td></td>
<td>1675.9x10$^3$</td>
<td></td>
</tr>
<tr>
<td>$T_{\text{sat}}$ [K]</td>
<td>500.7</td>
<td></td>
<td>530.0</td>
<td></td>
</tr>
</tbody>
</table>

Table 4-3: Mechanical and thermophysical properties of pressurised water.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>22.7 bar case</th>
<th>45 bar case</th>
</tr>
</thead>
<tbody>
<tr>
<td>LX [μm]</td>
<td>238.0</td>
<td>78.36</td>
</tr>
<tr>
<td>R0 [μm]</td>
<td>79.4</td>
<td>30.05</td>
</tr>
<tr>
<td>$\Delta t_0$ [ms]</td>
<td>5</td>
<td>1.295</td>
</tr>
<tr>
<td>$\Delta T$ [K]</td>
<td>6.13</td>
<td>6.13</td>
</tr>
<tr>
<td>Ja</td>
<td>0.966</td>
<td>0.627</td>
</tr>
</tbody>
</table>

Table 4-4: Physical parameters of test cases of spherical bubbles growing in isolation.

Specification of the initial temperature field in the liquid is more complex. The remote liquid is initially taken to be superheated by an amount $\Delta T = T_{\infty} - T_{\text{sat}}$. The computational model cannot start from a zero bubble radius. Whilst one would expect the influence of an arbitrary choice of initial conditions to decline rapidly, if the initial bubble size specified were small enough, it is sensible to use what we believe is a plausible set of initial conditions. This is done by taking one of the results due to Scriven, from which we can estimate the initial radius believed to obtain after some corresponding early time:

$$R_0 = 2\beta \sqrt{\alpha I \Delta t_0}$$  \hspace{1cm} (4.1)

The growth constant $\beta$ is computed via numerical integration, as discussed in Chapter 2.

The initial temperature distribution is evaluated based on the analytical solution obtained in the original work by Scriven. The expression for evaluating the temperature profile in the liquid as a function of distance from the interface - $T(R - R_0, \Delta t_0)$ - is as follows:
\[ T = T_\infty - 2\beta^2 \left( \frac{\rho_g (h_{fg} + (c_{pl} - c_{pg}) \Delta T)}{\rho_f c_{pl}} \right) \int_{1-R(t)/r}^1 \exp \left( -\beta^2 \left( \frac{1-\xi}{2} \right)^2 - 2\left( 1 - \frac{\rho_g}{\rho_f} \right) \xi - 1 \right) d\xi \]  

(4.2)

where \( \xi \) represents a dummy variable. This is specified as the initial temperature distribution.

### 4.2.2 Numerical issues

As explained in Chapter 3, curvature of the liquid-vapor interface is calculated from the signed distance function. For the present case of very small cavities with high curvature, the approximations associated with evaluating this in a discrete form contribute to causing spurious circulatory currents to be generated in the adjacent fluid. This is referred to in the following as original curvature calculation. However, for this particular study of spherical voids, we are able to use a particular, and very accurate, curvature value of \( 2/R \) (referred to in the following as improved curvature calculation), and this contributes greatly to their reduction (Yokoi (2013)).

The currents are caused because these normals appear in the surface tension term of the momentum balance equation. When there is little fluid motion (as in bubble growth at high pressure, which is rather slow compared to low pressure), the currents can pollute significantly the solution (particularly, in our case, the temperature distribution). Several approaches have been proposed to alleviate this problem. In this particular case, since the only fluid motion expected is radially outwards, with the original curvature calculation, we impose a high value of the viscosity (ten times the viscosity of the liquid phase) in both the gas and liquid to limit spurious currents. The value of the artificial viscosity was chosen based on numerical experiments: keeping a constant discretization, four cases with increasing viscosities were run, and the total kinetic energy in the computational domain was monitored. It was expected a divergent behavior of the kinetic energy for the real viscosity case, due to the unphysical build-up of a recirculation flow pattern caused by the spurious currents. On the other hand, the simulations with the artificial viscosities were not expected to show this behaviour. This trend actually emerges from Figure 4-11. The quantity plotted on the ordinate
is obtained evaluating half of the square of one component of the velocity vector (thanks to the spherical symmetry of the problem, it has no importance which component, namely, in this case, along the x-direction) and summing over all the computational cells. Thus the quantity obtained can be interpreted as a specific kinetic energy, with units \( \frac{1}{kg} = \frac{m^2}{s^2} \). The monitored quantity increases for two reasons: i) the initial build-up of the spurious recirculation and ii) after the recirculating pattern is established, the region of the domain affected by it – localized near the interface – increases in size due to bubble expansion. Following the numerical experiment described, a value of the viscosity equal to ten times the liquid viscosity is adopted for both phases.

![Graph](image)

Figure 4-11: Temporal evolution of kinetic energy for different values of artificial viscosity, computed for the case of a spherical bubble growing in isolation.

On the other hand, with the improved curvature calculation, use of the physical viscosity is made. However, in order to apply the present methodology to a broader range of problems, it will be necessary to adopt a different calculation of the interface curvature. In the following, we present results for three cases: i) original curvature calculation with real viscosity, ii) original curvature calculation with artificial viscosity, iii) modified curvature calculation with real viscosity.
4.2.3 Results

Results from a mesh independence study for the 22.7 bar case with the artificial viscosity are shown in Figure 4-12, where the analytical and numerically computed growth curves are plotted. Since the production of vapour is calculated based on the heat flux jump at the interface, the refinement is dictated by the need of resolving the thermal boundary layer in the water. Three cases of equal-spacing grid with different resolution – 48, 72 and 144 cells per side – have been tested. Convergence towards the analytical solution is observed if the artificial viscosity is used. On the other hand, with the physical viscosity, the computed bubble radius begins to depart from the analytical solution.
Figure 4-12: Top: mesh independence study for the 22.7 bar isolated bubble case with artificial viscosity. Bottom: growth rate obtained with the finest mesh with the real viscosity.

The difference in computed temperature and volumetric vapor production \( (kg/m^3s) \) fields after 8 ms between the real (fine mesh) and artificial (intermediate mesh) viscosity cases is shown in Figure 4-13. The actual numerical values of the computed temperature and volumetric vapour production fields are not relevant; what matters here is the shape. The spurious currents cause recirculating flow patterns near the gas-liquid interface that distort the temperature distribution in the liquid water. Since the production of vapor is calculated based on the temperature gradients in the water at the interface, non-uniform vapour production is predicted. It is seen that as a consequence of the increased viscosity, the intensity of the spurious currents is reduced and the large recirculation that appears near the bubble poles and equator if the real viscosity is used is damped. As a consequence, physically plausible temperature and volumetric vapor production distributions are obtained.
Figure 4-13: Results of the simulation of a spherical bubble growing in isolation, 22.7 bar case. Top panel: temperature (left) and volumetric vapor production distributions after 8 ms using the real viscosity; velocity vectors also shown. Bottom panel: Temperature (left) and volumetric vapor production (right) distributions after 8 ms using the artificial viscosity; velocity vectors also shown.

Growth rates obtained with an improved calculation of the interface curvature are shown in Figure 4-14, Figure 4-15 and Figure 4-16. Convergence towards the analytical solution is observed if the mesh is refined and better agreement with the analytical growth rate is observed with respect to both the real viscosity and artificial viscosity cases with the original curvature calculation. The temperature and volumetric vapor production predictions are also improved. The thermal boundary layer remains spherically symmetric, as a consequence of the disappearance of the recirculating areas near the bubble poles and equator. In addition, the abnormally high velocity vectors appearing at some locations along the interface if the fictitious viscosity is prescribed are no longer present.
Figure 4-14: Mesh independence study for the 22.7 bar isolated bubble case using the improved curvature calculation and physical viscosity.

Figure 4-15: Results of the simulation of a spherical bubble growing in isolation, 22.7 bar case. Comparison between growth rates obtained with the finest mesh using artificial viscosity (original curvature computation), physical viscosity (original curvature computation) and the improved curvature computation.
Figure 4-16: Temperature (left) and volumetric vapor production (right) distributions obtained for the 22.7 bar isolated bubble case after 11.75 ms using the real viscosity and improved curvature calculation.

The methodology described for the 27 bar case was also applied to the 45 bar case. Spurious currents, and their significant reduction if either of two remedies described above was adopted, were observed. The results will not be reproduced here (they add nothing); a discussion of the 45 bar case is however available in Giustini, Murallidharan et al. (2015).

4.3 High pressure wall boiling case

4.3.1 Experimental arrangements of Sakashita

The experimental arrangements devised by Sakashita (2011) were used to make photographic observations of steam bubble growth at pressures up to 45 bar. For present purposes, use is made of a data set collected during boiling of water at 45 bars at a horizontal surface. As for the atmospheric pressure benchmark described in the preceding text, the boiling surface is considered isothermal, its temperature assumed equal to the incipient nucleation temperature. For the case under investigation, the incipient nucleation temperature corresponds to a superheat of 1.83 °C above the saturation temperature and to a Jakob number of 0.18.
4.3.2 Computational model

The same physical model of section 4.1.2 is used, albeit with different numerical values of the bottom surface temperature, and of the initial superheated liquid layer thickness, respectively equal to 258.68 °C and 0.932 mm. The thermophysical properties of saturated water at 45 bars are used, Table 4-3. The input thermodynamic contact angle is set to 0°. Dimensions of the computational domain are shown in Figure 4-18. In the region where the bubble develops, a uniform discretization is adopted. Outside this region, the mesh is stretched in order to reduce computational cost. The minimum cell size is 3.125 micron, corresponding to a thermal penetration depth in the liquid after approximately 0.05 milliseconds, Figure 4-19. A total of 606,208 cells were used.
4.3.3 Spurious currents

As for the spherical bubble in isolation, the computed temperature distribution was affected by unphysical currents generated close to the bubble curved surface, as shown in Figure 4-20, where results obtained using the original curvature computation are shown.
Altering the fluid viscosity considerably reduced the spurious currents, and did not change significantly the computed bubble shape, as shown in Figure 4-21, showing results obtained using the original curvature computation and imposing in both phases a value of the viscosity equal to five times the liquid viscosity.

Figure 4-20: Temperature distribution around the bubble after 20 (top) and 50 (bottom) ms for the original curvature computation, in conditions of the experiments of Sakashita. Physical values of the liquid and vapour viscosities have been used.
Figure 4-21: Temperature distribution around the bubble after 20 (top) and 50 (bottom) ms for the original curvature computation, in conditions of the experiments of Sakashita. Artificially high values of the liquid and vapour viscosities have been used.

So far, the surface tension component of the body force term in the Navier-Stokes equations has been treated as in the original CSF formulation, described in Chapter 3. Significant spurious currents were generated, as shown by the illustrations above, unless an artificial viscosity was introduced to dampen the spurious flows. In order to treat the wall-boiling case with physical values of the viscosity, a density-scaled version (Sato and Ničeno (2015)) of the CSF model was used, whereby the surface tension force is computed as follows:
\[ f_s = \sigma \kappa \frac{\nabla \rho}{(\rho_l - \rho_v)} \frac{\rho}{(\rho_l + \rho_v)} / 2 \] (4.3).

Figure 4-22: Temperature distribution around the bubble after 20 (top) and 50 (bottom) ms obtained using a density scaled CSF model to compute the surface tension force. Conditions of the experiments of Šakashita. Physical values of the liquid and vapour viscosities have been used.

Spurious current appeared greatly reduced adopting this improved surface tension computation, Figure 4-22.
4.3.4 Discussion

4.3.4.1 Spurious currents

Time histories of equivalent bubble diameter are shown in Figure 4-23 for various viscosity-surface tension computation combinations. If the original surface tension computation is used (top left panel in Figure 4-23), a small discrepancy is observed between the growth curve obtained with the physical viscosity values, and that obtained imposing the artificial viscosity. Similarly, if the physical viscosity is maintained (top right panel), adopting the density-scaled CSF model causes a moderate change in the growth curve. Finally (bottom panel), a comparison between the growth curve obtained with the original curvature computation, for the case of fictitious viscosity, and that obtained with the density scaled CSF, for the real viscosity case, shows a marginal difference in computed bubble growth. Overall, the investigation leads to the conclusion that the computation of bubble development at high pressure is mildly affected by spurious currents, at least in the conditions here considered.

Figure 4-23: Influence of spurious currents on computed bubble growth during pool boiling at high pressure.
4.3.4.2 Comparison with analytical growth rate

The time history of equivalent bubble diameter was compared against predictions of the analytical model, as shown in Figure 4-24. Reasonable agreement is observed, although a small discrepancy, increasing with time, is present, perhaps due to the finite initial size of the bubble in the CFD simulation.

Figure 4-24: Comparison of bubble-growth curve from ITM analysis with the analytical growth curve, in high-pressure conditions.

This favourable comparison with an ‘exact’ solution indicates that the CFD methodology is capable of capturing correctly the steam formation mechanism at the bubble surface.

4.4 Concluding remarks

Results of the mechanistic CFD modelling described in this chapter prompt the following remarks:

- Scriven-type solutions for the time-dependent bubble growth rate agree well with predictions of CFD analyses that do not include evaporation microlayers. This has been shown to be the case for pool-boiling test cases characterized by low (up to 18) Jakob numbers.
• Bubble expansion at a heated wall at atmospheric pressure was predicted with good agreement with experimental data. Microlayer evaporation was not included in the model, which suggests, a posteriori, a minor influence of this mechanism of vapour production on bubble formation at Jakob numbers similar to those here considered.

• The simulation of bubble formation in high-pressure conditions was found to be affected by numerically generated spurious currents. Two methods to alleviate this issue have been tested, capable of reducing considerably the currents.

• The prediction of bubble growth rates was found to be weakly affected by the spurious currents, even though such currents had a macroscopic influence on the details of the flow close to the bubble-curved surface.
CHAPTER 5
EVAPORATIVE THERMAL RESISTANCE, AND ITS INFLUENCE ON STEAM BUBBLE GROWTH

In this chapter, the notion of an equivalent heat transfer coefficient, associated to interphase mass transfer at the vapour-liquid interface, is introduced. Use is made of the commonly accepted representation of the phenomenon in order to show its insignificance as regards evaporation at the bubble-curved surface. On the other hand, via analysis of a recent set of measurements, it is demonstrated that microlayer evaporation rates are influenced by evaporative heat transfer coefficient values. Moreover, the thermal resistance associated to the evaporation process is shown to be significant, and often much larger, than that offered by the liquid film itself. This is shown to be the case regardless of the thermal properties of the substrate; in other words, that evaporative resistance is significant not just for the case of microlayers evaporating from highly conductive substrates.

5.1 Background: current modelling of bubble-curved surface and microlayer evaporation

It will be recalled from the previous chapter that, as a steam bubble grows at a heated substrate, a microlayer of liquid is observed to be left beneath it, Figure 2-1. Being such a thin (micrometric) layer, the flow of heat through it is large. This is because heat flow is driven by the temperature difference between the substrate-liquid interface and the liquid-vapour interface, and this difference exists over a very small distance. Consequently, the micro-layer is believed to be responsible for a significant fraction of the vapour generation under many circumstances, such as the boiling of atmospheric water at a superheat around 10 K. In such conditions, its radial extent is a few hundreds of microns, and its thickness a few microns, increasing slightly with radial distance from the nucleation site. It is believed that there is essentially no flow of liquid into or out of the micro-layer, and thus its evaporation results in its thickness reducing, and the eventual disappearance of the layer. Since this occurs first at its inner radius, where the initial thickness of the film was least, there is an associated progressive increase in the radius of the dry patch around the nucleation site (Kim and Buongiorno (2011)).
As discussed in Chapter 2, the evaporation from the curved surface is limited by the rate at which heat diffuses across the relaxation layer. The normal heat flux so computed in the liquid is used to determine a corresponding rate of vaporisation, and a corresponding vapour flux into the bubble.

The usual approach to modelling heat transfer through and vaporisation from the micro-layer is to treat it as a thin film, through which the heat flux is determined by its upper and lower surface temperatures, and where this heat flux in turn is used to compute the local vapour generation rate. This rate is used both to contribute to the increasing bubble volume, and to compute the gradual thinning and eventual disappearance of the micro-layer from the centre outwards.

Figure 5-1: our current understanding of the microlayer.

5.2 Evaporative thermal resistance

In the above discussion, for both the main curved surface of the bubble and for the micro-layer, the taking of the vapour-liquid interface temperature to be equal to the saturation temperature is equivalent to assuming that the evaporative heat transfer process is “infinitely effective”, or equivalently can be modelled by an infinite value of heat transfer coefficient.
Some temperature difference is actually required to drive the flux of molecules from the liquid into the vapour. Expressing this in terms of an ‘evaporative heat transfer coefficient’, its value is indeed usually large, and the resistance to heat transfer it represents is a tiny fraction of the other resistances involved (such as the diffusive resistance impeding flow of heat from the bulk liquid to the bubble).

However, the thermal resistance of a thin micro-layer is itself small, and becomes vanishingly small as it thins. If the micro-layer plays a significant role in bubble development, neglect of the evaporative resistance might be expected to have a measurable influence on its contribution to predicted bubble growth.

In this chapter we focus on the micro-layer during nucleate boiling of water at atmospheric pressure and investigate the significance of the inclusion of the evaporative thermal resistance.

5.2.1 Evaporation from a molecular point of view

A liquid surface exposed to its vapour is considered, shown in Figure 5-2. Even in conditions of no net evaporation or condensation, the interface is in a state of dynamic equilibrium, whereby a continuous stream of molecules impinges on it from the vapour. Similarly, molecules are continuously emitted from the surface. It is initially assumed that all vapour molecules impinging on the surface are absorbed, and that all the molecules emitted from the surface are transferred to the vapour. If the temperature and pressure of the vapour are known, with kinetic theory of gases it is possible to determine the rate of deposition of molecules from the vapour onto the surface. At equilibrium, i.e. a condition of no net interphase mass transfer, the rate of deposition must equal the rate of emission from the surface. This allows determining the equilibrium rate of emission, known the liquid temperature. The emitted flux can be expressed as a function of the saturation pressure, at the liquid surface temperature, of the vapour phase of the substance undergoing phase change, and the impinging flux as a function of the vapour pressure.
However, the assumption that all impinging molecules ‘stick’ to the surface is not justified. In fact, according to current understanding of the molecular mechanism of interphase mass transfer, reflections occur. The implication is that, of the molecules transferred to the vapour, some are those actually emitted from the liquid, and the remainder are those reflected. This is illustrated in Figure 5-3.

5.2.2 Extant evaporative heat transfer coefficient treatment (Schrage’s theory)

We follow here the development in Schrage (1953). Assuming that the vapour is an ideal gas and that the velocities of the molecules in the impinging and escaping fluxes follow a Maxwellian distribution (steady state assumption), from the kinetic theory of gases one can obtain the following expression for the flux of molecules from the vapour, impinging on the liquid surface:
\[
\dot{m}_v'' = \frac{p_v}{\sqrt{2\pi R T_v}}
\]  

and, as explained in the preceding text, to the vapour:

\[
\dot{m}_l'' = \frac{p_l}{\sqrt{2\pi R T_l}}
\]

where \(p_l\) and \(p_v\) are the liquid and vapour pressures, and \(T_l, T_v\) the liquid and vapour temperatures. Knudsen estimated the net flux as the difference between the two (Knudsen (1915)). However, Schrage showed that this is not adequate for two reasons:

i) Of the molecules transferred to the vapour, a fraction \(f_e\) is actually due to emission from the liquid, the remaining part \(1 - f_e\) being impinging molecules reflected back. The other side of the coin is that only a fraction \(f_e\) of the impinging molecules gets adsorbed in the liquid. Therefore, the net flux is \(f_e \dot{m}_l'' - f_e \dot{m}_v''\).

ii) There is an additional factor to consider including; an allowance for the bulk motion of molecules towards the liquid during condensation, or away from it during evaporation. From Tanasawa (1991), this is given by:

\[
\Gamma = 1 \pm \frac{\dot{m}_l''}{p_v \sqrt{\frac{2}{\pi R T_v}}} \]

where \(\dot{m}_l''\) is the net mass flux across the interface, and the + sign applies to condensation, while the sign – applies to evaporation. For atmospheric water at a condensation rate corresponding to a heat flux of 1 MW m\(^{-2}\), not untypical of micro-layer heat fluxes, the second term on the right hand side of equation (5.3) is approximately equal to 0.002. Plainly for the cases of immediate interest it matters little, but it could perhaps become important under other circumstances.

Assuming this factor \(\Gamma\) to be equal to one, for the case of evaporation the net flux of molecules from liquid to vapour is given by

\[
\dot{m}' = f_e \dot{m}_l'' - f_e \dot{m}_v''
\]
At equilibrium, the same Maxwellian distribution must be maintained in the vapour, and no net mass flux is present. The first assumption implies that $\dot{m}''_e = \dot{m}''_v$, the second is expressed algebraically as $\dot{m}'' = 0$. Hence, at equilibrium

$$f_e = f_c = f$$

(5.5).

Following Schrage, we term $f$ an ‘evaporation coefficient’, and assume that the above equality holds also when net mass transfer is present. Taking $p_{lv}$ as the saturation pressure at the liquid surface temperature, the net mass flux can now be written as

$$\dot{m}'' = f \left( \frac{p_{SAT}(T_l)}{\sqrt{2\pi R T_l}} - \frac{p_v}{\sqrt{2\pi R T_v}} \right)$$

(5.6).

We will return to this expression later in the context of inferring a value for $f$. Under the assumption that the temperature difference between the liquid surface and the vapour is small compared to their absolute values, one can use the Clausius-Clapeyron relation $\frac{p_{lv} - p_v}{T_{lv} - T_v} = \frac{\rho_l h_f}{T_v}$ to obtain the following expression for the net mass flux across the interface as a function of fluid properties and interface superheat:

$$\dot{m}'' = \frac{h_f \rho_v (T_v - T_l)}{T_v \sqrt{2\pi R T_v}} f$$

(5.7).

The mass flux in this expression is readily converted into a heat flux. We will express the resulting relationship between interface superheat and heat flux via the evaporative thermal resistance

$$T_v - T_l = \frac{T_v \sqrt{2\pi R T_v}}{h_g \rho_v f} \dot{q}''$$

(5.8).

If the vapour is assumed to be at the saturation temperature at the system ambient pressure we then have
\[ T_l - T_{SAT} = \frac{T_{SAT} \sqrt{2\pi R T_{SAT}}}{h_f \rho \gamma f} \dot{q}'''' = \frac{1}{h_{ev}} \dot{q}'''' \] 

This provides an estimate for the evaporative heat transfer coefficient:

\[ h_{ev} = \frac{h_f \gamma \rho}{T_{SAT} \sqrt{2\pi R T_{SAT}}} f \]  

(5.10)

Its value is seen naturally to depend on the fluid properties, and in particular on the evaporation coefficient and the latent heat of evaporation.

Equation (5.7) tells us that, during both evaporation and condensation, the mass flux across the interface is driven by a temperature difference between the liquid surface and the vapour adjacent to the surface. For example, when the liquid side of the interface is hotter than the gas side, there is a net flux of molecules leaving the liquid and entering the gas because of this temperature difference. From a molecular point of view, this temperature difference, albeit presumably very small, is present even in the case of ‘perfect’ emission and absorption of molecules from the liquid surface. The term ‘perfect’ here denotes circumstances when all the molecules impinging the liquid surface are absorbed \((f = 1)\). In general, not all the molecules impinging on the surface are captured, as some are reflected back \((f < 1)\). At equal temperature difference, this means that a higher temperature difference is required to attain an equal evaporation rate.

### 5.3 Typical evaporative heat transfer coefficient values

Considerable difficulties are encountered when trying to measure the evaporation coefficient. This can be done only indirectly, for example by measuring the temperature of the liquid surface, and inferring the coefficient. Usually, favourable conditions to measure the evaporation coefficient are present when the gas phase is sufficiently rarified. For the case of water, this means that most of the measurements of the evaporation coefficient are at low pressures (tenths or hundredths of bars), and hence there is paucity of measurements of the evaporation coefficient for pressures equal to or above atmospheric. In addition, there is a large scatter of values suggested for the evaporation coefficient (Marek and Straub (2001)),

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due to the diverse experimental arrangements devised to infer values of it. In the analysis presented here, based on a survey of the literature (Prueger (1940), Schrage (1953), Delaney, Houston et al. (1964), Tanasawa (1991), Marek and Straub (2001)), we will consider a large - but it seems fairly bounding - range of evaporation coefficients, namely between 0.01 and 1.

As discussed, the value of $f$ is rather uncertain, and we will now attempt to give a sense of the significance of this uncertainty. In Figure 5-4 we show the evaporative heat transfer coefficient $h_{ev}$ for water at atmospheric pressure, and, in terms relevant to the micro-layer, express this also as the thickness $\delta_f$ of a film of water offering an equal thermal resistance. Based on measurements reported in previous analyses (Marek and Straub (2001)), a plausible value for the evaporation coefficient is approximately 0.1. Using this value, for water at atmospheric pressure the evaporative heat transfer coefficient is about 1 MW m$^{-2}$ K$^{-1}$. The associated thermal resistance is equal to that presented by a film of liquid water of thickness 1.0 micron.

![Figure 5-4: The evaporative heat transfer coefficient for water at atmospheric saturation conditions (left axis), and expressed as the thickness of water film of equivalent thermal resistance (right axis), as a function of the evaporation coefficient.](image)

Another way to look at the interface thermal resistance is considering the interface superheat $S$ required to evaporate a given mass flux, Figure 5-5.
For steam - water boiling at atmospheric pressure, a typical value of surface mass flux might be about 0.01 kg/m²s for the evaporation rate at the bubble curved surface, with micro-layer fluxes more than fifty times this, perhaps 0.5 kg/m²s (Jung, Chung et al. (2015)). With an evaporation coefficient of 0.1, the interface needs to be superheated by a negligible 0.03 K in order to attain an evaporation rate representative of evaporation at bubble surface. This suggests that the interface resistance can be ignored when modelling evaporation at the bubble surface, which is the common approach. However, interface resistance causes a superheat of approximately 1.5 K to be required to attain fluxes typical of micro-layer evaporation.

**Figure 5-5**: Interface superheat per unit mass flux, for water at atmospheric pressure as a function of the evaporation coefficient.

### 5.4 Importance of the evaporative thermal resistance during bubble growth

We now focus on the importance of the evaporative thermal resistance during bubble growth, and provide an order of magnitude argument in order to assess its importance as regards the two evaporation processes discussed in preceding text.
5.4.1 Evaporation at the bubble-curved surface

For evaporation at the bubble surface, the thickness of the relaxation thermal layer increases with time, and is given by Plesset and Zwick (1954):

\[
d_{\tau}(t) = \frac{R(t)}{\left(\frac{\rho_{l}c_{p}\Delta T}{\rho_{v}h_{fg}}\right)} = \frac{R(t)}{Ja} \quad (5.11),
\]

where \( R(t) \) is the bubble radius. The denominator may be recognized as the Jakob number, \( Ja \).

The temporal variation of bubble radius can be obtained from the asymptotic solution for diffusion controlled bubble growth, here shown again for clarity:

\[
R(t) = Ja\left(\frac{12}{\pi}\alpha_{l}t\right) \quad (5.12).
\]

This gives the time dependent relaxation thickness as:

\[
d_{\tau}(t) = \sqrt{\frac{12}{\pi}\alpha_{l}t} \quad (5.13).
\]

We then identify the ratio between evaporative thermal resistance and thermal resistance of the relaxation layer that opposes the flow of heat into the bubble as

\[
\Omega = \frac{\frac{1}{h_{\text{ev}}}}{d_{\tau}(t)} = \frac{1}{h_{\text{ev}}} \frac{1}{d_{\tau}(t)} = \frac{1}{h_{\text{ev}}} \frac{12}{\pi \rho_{l}c_{p}\lambda_{l}} t \quad (5.14).
\]

This expression is plotted in Figure 5-6, where the symbol \( \Omega \) denotes the ratio (evaporative thermal resistance)/(thermal resistance of the relaxation layer).
Figure 5-6: Evaporation at the bubble surface: The ratio (vertical axis) between evaporative thermal resistance and thermal resistance of the relaxation layer as it varies with time during bubble growth, for various evaporation coefficients.

Even for the smallest evaporation coefficient considered, the evaporative resistance declines rapidly to less than 10% of the total resistance. Typical bubble growth times for water at atmospheric pressure are of order hundredths of seconds, and the time for which the evaporative thermal resistance is the dominant resistance to the flow of heat into the bubble is very much smaller. This suggests that the effect of the evaporative resistance should be considered only during the very early stages of bubble growth. A similar conclusion was reached by Bornhorst and Hatsopoulos (1967) via a different approach.

5.4.2 Evaporation from the microlayer

We now consider micro-layer heat transfer during the boiling of water at atmospheric pressure. Since the micro-layer thickness generally does not exceed five microns, the microlayer could offer resistance to heat transfer by conduction that is comparable to the evaporative resistance.
The ratio between the evaporative thermal resistance and the micro-layer thermal resistance is plotted in Figure 5-7 as a function of film thickness, for a range of values of evaporation coefficient. This shows clearly that as the micro-layer thickness decreases, the evaporative resistance becomes increasingly important.

5.5 Measured microlayer evaporation rates; the pool boiling test case of Jung and Kim

In what is perhaps one of the most comprehensive sets of measurements of bubble nucleation and growth, Jung and Kim (2014) and Jeong, Jung et al. (2015) reported detailed measurements of the thickness and radius of the micro-layer as it varied during the bubble growth process. These provide an excellent basis for the investigation of the significance of the evaporative resistance in modifying evaporation rates.

The working fluid is water, boiled at atmospheric pressure using a 700 nm thick Indium-Tin Oxide (ITO) film heater deposited on top of a 10 mm thick calcium fluoride substrate. The ITO heater surface is 8mm x 15mm, with the boiling chamber a cylinder of base diameter 50mm. The average heat flux over the heater is 200 kW/m².
This set of measurements clearly demonstrated the existence of the micro-layer beneath a vapour bubble growing in water at atmospheric pressure. Jung and Kim were able to measure bubble shapes, micro-layer profiles and the temperature distribution on the underside of the ITO layer by means of, respectively, synchronized high speed imaging, laser interferometry and infrared thermometry; see Figure 5-8. Full details of the measurements are available in Jung, Chung et al. (2015).

Figure 5-8: schematic of Jung and Kim’s experimental arrangements for measuring bubble-growth, microlayer geometry and the temperature at the solid-fluid interface.

5.5.1 Jung and Kim microlayer measurements

For present purposes the most important measurements are the series showing the development of the micro-layer. Results are presented of the radial variation of micro-layer evaporation rate, expressed as the rate of micro-layer thickness reduction, at a series of times. These measurements were obtained by two independent means:-

(i) Under the assumption that the liquid in the micro-layer is stagnant, optical interferometry allows the radial variation of micro-layer thickness to be measured directly at sequential times.

(ii) Measurement of the solid-liquid interface temperature through time allows the time-dependent variation of the surface heat flux in the solid substrate to be determined by highly accurate finite element “post-processing” of the temperature field within the substrate. On the
assumption that all of this surface heat flux goes into evaporating the micro-layer at the same location, the rate of thinning of the micro-layer can be determined.

(iii) A third ‘derived’ assessment of micro-layer thickness is also presented. Given the measurement of the solid surface temperature and the micro-layer thickness, and the assumption that the micro-layer upper surface temperature was equal to the saturation temperature, the heat flux through the micro-layer can be determined. From this the evaporation rate, and the rate of thinning of the micro-layer, can thereby be computed.

We reproduce here in Figure 5-9 these measured quantities, showing the micro-layer depletion rate assessed by the two direct measurements, and the third inferred method.

We will for brevity term these respectively:-

- Evaporation Heat Flux (i)
- Wall heat Flux (ii)

and the derived

- Conduction Heat Flux (iii).

The two independent measurements (i) and (ii) are in very good agreement with each other. For present purposes the other noteworthy feature of this graph is that the micro-layer depletion rate assessed by Method (iii) becomes inconsistent with the other two approaches at small radii, where the micro-layer is thin.

As discussed above, it is under these conditions that one would expect the neglect of surface evaporative resistance to begin to be significant. We will investigate whether or not inclusion of this phenomenon will restore consistency to the three approaches in the next section.
Figure 5-9: Reproduced from Jung, Chung et al. (2015). This shows the radial variation of micro-layer depletion rate reported by Jung and Kim, using the three different approaches discussed above. From top to bottom, the instantaneous micro-layer depletion profiles are shown at 1, 4 and 7 ms after bubble nucleation.
5.6 Re-evaluation of the microlayer heat flux radial and temporal variation incorporating evaporative thermal resistance

We can re-evaluate the heat flux via ‘Method (iii)’, but taking the evaporative thermal resistance into account, using the following expression:

\[
q''(r, t) = \frac{T_s(r, t) - T_{SAT}}{\delta(r, t)} + \frac{1}{h_{ev}}
\]

(5.15)

where \(T_s(r, t)\) is the local instantaneous value of the solid-liquid interface temperature and \(\delta(r, t)\) is the micro-layer thickness at radius \(r\) and time \(t\). This is done for values of evaporative resistance and evaporation coefficient listed in Table 5-1, taken from the range of values believed to be credible, and results for the three times are shown in Figure 5-10.

<table>
<thead>
<tr>
<th>Case</th>
<th>Evaporative resistance [m²K/W]</th>
<th>Evaporation coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td>hev1</td>
<td>1.275×10⁻⁷</td>
<td>1.00</td>
</tr>
<tr>
<td>hev2</td>
<td>1.275×10⁻⁶</td>
<td>0.10</td>
</tr>
<tr>
<td>hev3</td>
<td>1.275×10⁻⁵</td>
<td>0.01</td>
</tr>
</tbody>
</table>

Table 5-1: Values of evaporative resistance considered in the parametric study on the influence of ‘imperfect evaporation’ on microlayer depletion.

It is seen that inclusion of the effect indeed can restore consistency between the ‘derived’ and the two independent ‘measured’ results, and that a value of \(f\) lying between 0.1 and 0.01 seems appropriate. The very high value of heat flux predicted by Method (iii) close to the dry patch (where the micro-layer is becoming very thin) decreases significantly with progressively larger values of evaporative resistance.
Figure 5-10: influence of evaporative resistance on microlayer depletion.
5.7 Inferring of evaporation coefficient value

In the discussion above we employed a range of values of evaporation coefficient, and inferred by inspection a plausible value. In this section we will approach this more systematically, and compute directly the value required to generate a ‘derived’ heat flux consistent with the two measurements. (Note, of course, that as the two measurements are naturally not perfectly consistent with each other, the consistency of the derived approach has a similar degree of tolerance).

The approach adopted is:-

Knowing the wall temperature and the heat flux, the micro-layer upper surface temperature is computed:

\[
T_{lv}(r,t) = T_{sr}(r,t) - \frac{\delta(r,t)q''(r,t)}{\lambda}
\]  

(5.16).

Using this temperature, the evaporative resistance is computed:

\[
\frac{1}{h_{ev}} = \frac{q''}{T_{lv} - T_v}
\]  

(5.17).

The evaporation coefficient is inferred (using equation (5.6)), assuming the vapour at the saturation temperature at the system ambient pressure \(p_{ref}\):

\[
f_{inferrd} = \frac{\frac{p_{SAT}(T_v)}{p_{ref}}}{\sqrt{\frac{2\pi RT_v}{p_{ref}}}} - \frac{2\pi RT_{SAT}(p_{ref})}{\sqrt{2\pi RT_{SAT}(p_{ref})}}
\]  

(5.18),

where the saturation pressure at the interface temperature is computed according to the perfect gas law:

\[
p_{SAT}(T_v) = p_{ref} \exp \left[ \frac{h_l}{R} \left( \frac{1}{T_{SAT}(p_{ref})} - \frac{1}{T_v} \right) \right]
\]  

(5.19),

and \(p_{ref} = 101325\) Pa (vapour assumed at system ambient pressure) and \(T_{SAT}(p_{ref}) = 373.15\) K.
We have used this approach to compute the evaporative thermal resistance needed for consistency at each measurement location, at each time. Values are shown in Figure 5-11. Note that one would expect this assessment to become less well conditioned in regions where the micro-layer is thicker, and the evaporative thermal resistance is correspondingly a smaller fraction of the total thermal resistance. More weight should thus perhaps be given to values towards the inner radius.

![Evaporative resistance graph](image)

Figure 5-11: value of the evaporative thermal resistance inferred from experimental data at 1, 4 and 7 ms after bubble nucleation.

In any event, it seems reasonable to infer a value of evaporative thermal resistance between $2 \times 10^{-6}$ and $10 \times 10^{-6}$ m$^2$K/W. At small radii, where the micro-layer is thinner (and thus evaporative resistance more important), very similar values of evaporative resistance are obtained at each of the three times considered (respectively, 5, 7 and $8 \times 10^{-6}$ m$^2$K/W), an indication of the robustness of the present approach.
Evaporation coefficient inferred from experimental data at 1, 4 and 7 ms after bubble nucleation.

The approach can be repeated, to estimate a plausible range of values for the evaporation coefficient itself (Figure 5-12), giving corresponding approximately bounding values 0.02 and 0.1. These values are indicated on the figure (black lines). The evaporation coefficient inferred with measurements from to points close to the inner micro-layer radius is very similar at each of the three times considered, and close to 0.02.

The degree of non-uniformity with respect to both location and time is quite significant, and seems to be greater than, for example, mere experimental uncertainty might cause to be seen.

As discussed above, the basic concept of ‘evaporation coefficient’ by construction corresponds to the assumption that the evaporative process is able to be described by a ‘evaporative heat transfer coefficient’, relating the heat flux linearly to the difference between the liquid surface temperature and the bulk vapour (saturation) temperature. One possible explanation would be if the evaporative process were not actually able to be so described, but rather displays a different dependence on this temperature difference. This is an interesting possibility, as it would cast doubt on the ‘evaporation coefficient’ approach, and it thus seems an area requiring further investigation.
Using bounding values for $f$, 0.02 and 0.1, we now show in Figure 5-13 an indication of the ratio ‘evaporative / conductive’ in the resistance to the flow of heat that is presented by the micro-layer. It is seen that even for the higher evaporation coefficient (the dots), the evaporative resistance would be everywhere a significant contributor to the total thermal resistance. For the lower value (solid lines), evaporative resistance dominates the conductive. This suggests strongly that in general the sub-grid micro-layer models used in bubble growth modelling should be augmented to include this effect.

![Figure 5-13: The microlayer evaporative resistance relative to the conductive resistance at each of the three times, for the upper (points) and lower (solid lines) bounds to the evaporation coefficient.](image)

**5.8 Discussion**

Microlayer evaporative resistance is generally not included in microscopic modelling of vapour bubble growth. However, it has been shown to be important in some circumstances, and in particular in the understanding of the evaporation of the micro-layer beneath the bubble. For many conditions, micro-layer evaporation is a significant contributor to the vapour forming the bubble. Therefore, inclusion of evaporative thermal resistance is required in the formulation of a proper microlayer depletion model for use in CFD simulations of steam bubble development.
So far, it has been demonstrated that evaporative resistance is comparable to - if not larger than – the conductive resistance of the water film. However, assessing the absolute importance of evaporative resistance in the system solid-film-vapour requires taking into account the thermal resistance of the solid. The physical model used to do so is shown in Figure 5-14.

![Physical model and electrical analogy used in the assessment of the importance of evaporative resistance in the system solid-film-vapour, used to represent microlayer depletion.](image)

We assume that a thermally thick solid substrate, initially at a uniform temperature $T_{\infty}$, is initially in contact with a liquid film of thickness $\delta_{avg}$, also initially at $T_{\infty}$. The vapour is at the saturation temperature $T_{SAT}$. In the figure, an indicative temperature distribution is shown, representative of a little time into the cooling transient.

The series of thermal resistances is:

$$P_s \approx \frac{\delta_m}{\lambda_s} = \sqrt{\frac{l}{\lambda_s c \rho_s}} = \frac{\sqrt{l}}{\varepsilon_s},$$

$$P_l = \frac{\delta_{avg}}{\lambda_l},$$

$$P_{ev} = \frac{1}{h_{ev}},$$

(5.20)
We consider the typical case of $\delta_{avg} = 2 \mu m$ and $r_{ev} = 6 \times 10^{-6} m^2 K/W$ and vary parametrically the thermal properties of the substrate. (We will return to this model in Chapter 7, whereby depletion of the layer will be properly taken into account). Two limiting cases of high thermal conductivity (copper) and low thermal conductivity (calcium fluoride) materials are considered. However, in transient conduction heat transfer, also the thermal capacity contributes to determining the time-dependent thermal resistance. Thermal capacity features in the expression for the solid thermal resistance at the denominator, which is recognised as the thermal effusivity. The cases here considered correspond respectively to thermal effusivities of $37192.6 s^{1/2}/m$ and $3862.5 s^{1/2}/m$. This simple model clearly indicates that evaporative thermal resistance can be much larger than the conductive thermal resistance of the substrate, Figure 5-15, for the case of good conductors. Also for poor conductors, evaporative resistance is non-negligible when compared to the resistance of the substrate.

In passing, we note how this fact might be at the origin of the extreme importance attributed to microlayer evaporation by the analysis of Cooper and Vijuk (1970), the basis of the model of Sato and Ničeno (2015), due to its neglecting evaporative resistance.
Figure 5-15: temporal evolution of the thermal resistances involved in the solid-film-vapour system used to represent microlayer depletion. High- and low- thermal effusivity substrates are considered.
CHAPTER 6
KINETIC ANALYSIS OF MICROLAYER EVAPORATION

In this chapter, attempts at modelling microlayer evaporation from a molecular point of view are described. The starting point is the analysis of measurements of microlayer depletion. A model of evaporation is proposed, based on a simple kinetic theory representation of the molecular fluxes impinging on and emitted from a liquid surface, and shown incapable of producing results in agreement with measured evaporation rates. Neither the application of a more accurate model, based on the Boltzmann equation, is able to resolve the inconsistency. If the hypothesis, that only a fraction of impinging molecules are absorbed by a liquid surface, is introduced, better agreement is obtained. The chapter closes with speculations about the implications of this partial sticking hypothesis.

6.1 Experimental observations of microlayer evaporation

6.1.1 The experiment

The detailed microscopic experiments of Jung, Chung et al. (2015) were aimed at understanding the bubble growth process in general. The aspect that is relevant here was the detailed measurement of the depletion of the microlayer. Whilst heat fluxes through it are fairly high (order of one megawatt per square meter), they are by no means unusual from an engineering point of view, and are lower, for example, than some single phase convective heat fluxes in water. The important point for present purposes is that, as will be seen later, the evaporative process itself represents an unusually large fraction of the overall resistance to heat transfer.

The depletion of and heat transfer through this microlayer was measured using optical and infrared techniques, as indicated in Figure 6-1. Optical measurement of the film thickness at sequential times and various positions allowed direct evaluation of the rate of depletion of the liquid layer, and of the corresponding heat flux. A second assessment of the film depletion rate made use of infrared measurements of the spatial and temporal variation of the temperature at the solid-liquid interface. The measurements were used as time-dependent boundary conditions for a finite element model of the unsteady temperature distribution in
the solid, which allowed evaluation of the heat flux at the solid-liquid interface. From this the evaporation rate can be determined. These are very small scale, short duration events, and within the understandable experimental uncertainties these independent measurements were in broad agreement.

Figure 6-1: Independent measurements of observable quantities related to microlayer evaporation: optical interferometry measurement of the film thickness, and infra-red measurement of the temperature at the solid-liquid interface.

6.1.2 The anomaly

A third derived assessment of microlayer heat flux / depletion rate that was reported made use of the measurements of the temperature at the solid-liquid interface, and of the film thickness.
Figure 6-2: The model implicit in the derived assessment of the heat flux associated to microlayer depletion, showing the temperature variation from the deep solid through to the remote vapour.

The physical model implicit in this derived assessment of microlayer depletion rates is shown in Figure 6-2. Taking the temperature at the upper surface of the microlayer – the liquid-vapour interface – as the remote vapour temperature, and this to be the saturation temperature at the prevailing (atmospheric) pressure, the heat flux was computed as quasi-steady conduction through the film:

\[ q'' = h'' \dot{m}'' = \frac{T_s - T_{sat}}{\delta \lambda} \]  \hspace{1cm} \text{(6.1)}

This implicitly treats the evaporation process as ‘perfect’, and as offering no resistance to this flow of heat or mass. The variation of the heat flux obtained via the three different methods is plotted against the film thickness in Figure 6-3. The red circles are based on the direct evaluation of microlayer depletion via sequential optical measurements of film thickness. The blue diamonds show the heat flux obtained via post-processing of the unsteady temperature distribution in the substrate. Finally, the black squares indicate the third, ‘derived’ assessment of the microlayer depletion rate via equation (6.1). It is clear that at small film thicknesses
there is a considerable discrepancy between the two, reasonably consistent, measurements and the derived values.

Figure 6-3: The inconsistency between the two independent measurements of heat flux, and the assessment of heat flux derived from the evaporation model (‘Derived’).

6.1.3 Resolving the inconsistency

In Giustini, Jung et al. (2016) the physical model of the solid-film-vapour system was augmented to include arbitrary ‘imperfect’ evaporation at the upper surface of the microlayer, with this imperfection being characterised via an ‘evaporative heat transfer coefficient’, $h_{ev}$.

The flow of heat, and the evaporation rate, are then given by an augmentation of (6.1):

$$\dot{q}' = h_{ev} \dot{m}' = \frac{T_d - T_{SAT}}{\delta + \frac{1}{\lambda/ h_{ev}}}$$  \hspace{1cm} (6.2).

This expression was evaluated using different evaporative heat transfer coefficients, varied as a free parameter. It was shown that appropriate choice of the evaporative heat transfer
coefficient is able largely to eliminate the inconsistency between the derived and measured microlayer depletion rates. Comparison between the original measurements and values of the heat flux obtained with the physical model including evaporative heat transfer is shown in Figure 6-4. There, ‘hev1’, ‘hev2’ and ‘hev3’ indicate the three values of evaporative heat transfer coefficient considered, equal respectively to 7,500,000, 750,000 and 75,000 W/m²/°K.

Figure 6-4: Restored consistency in heat flux assessment via introduction of evaporative heat transfer coefficient.

6.2 Analysis

6.2.1 The approach adopted

In this section, attempts to interpret and understand this behaviour in the context of various simple kinetics models of gas behaviour and evaporation are described.

The first treatment below, in Section 6.2.2, is based upon a very simple kinetic model, where all impinging vapour molecules are assumed to be absorbed into the liquid. This is indeed, in broad terms, the conclusion of various studies of this process (Rose (2015)). It is also helpful as a starting point for the subsequent assessments where less than total ‘sticking’ is assumed. This first approach also serves as a vehicle by which we can explore a mechanism that has been proposed by Bornhorst and Hatsopoulos (1967). This based on the suggestion that the
free liquid surface is hotter than the bulk vapour, resulting in a flow of heat, and hence evaporative mass flux, lower than if the interface were maintained at the saturation temperature.

The second approach broadly mirrors the "simple kinetics" aspects of the first, but it incorporates the assumption that not all vapour molecules impinging upon the liquid surface enter the liquid (Schrage (1953)).

The third approach, termed here the ‘jump coefficient’ approach, is based on a suggestion of Sone and Onishi (1978), where there is postulated to be a jump in the temperature at the liquid – vapour interface, with the size of the jump determined from consideration of the speed distribution of the gas molecules.

6.2.2 Analysis based on simple kinetic theory

6.2.2.1 Postulated model, terminology & notation

The uniform pressure throughout the system \( p_{sys} \) is taken to be set by external means (such as the atmosphere for pool boiling, possibly augmented by surface tension effects for small enough bubbles, or by the pressuriser in a nuclear reactor). As noted, we incorporate, in order to investigate it, the possibility that the vapour temperature immediately adjacent to an evaporating surface will be slightly above the ‘remote’ vapour temperature. From here the temperature then falls to this remote value after some small distance (albeit a distance taken to be long compared to the molecular mean free path). Commonly, if the boiling is into saturated liquid, and as is the case in the experiments at issue, the remote vapour temperature would be the saturation temperature at the externally-imposed system pressure, \( T_{remote} = T_{sat}(p_{sys}) \), and this will be assumed here. The heat leaving the solid will mostly be ‘lost’ in forming vapour at the liquid-vapour interface. Incorporating the suggestion noted above, some additional sensible heat will be lost, via transfer of heat onwards to the bulk vapour.
6.2.3 Heat balance

The heat flow from the solid-liquid interface to the liquid-vapour interface is computed assuming quasi-steady heat conduction in the film as $\lambda_l \frac{T_{sI} - T_{lv}}{\delta}$. As noted, the vast majority of this heat is expended in the production of vapour at the liquid-vapour interface, while a presumably tiny fraction of it is transferred from the liquid to the vapour as sensible heat. If the temperature $T_{lv}$ at the liquid-vapour interface were known, we could compute directly the total (latent plus sensible) flow of heat. However such a temperature is not known a priori, and has to be computed via consideration of the molecular mechanism of evaporation, as follows.

The heat balance for the heat flowing through the liquid film out into the remote vapour at $T_{sat}(p_{sys})$ gives:

$$\frac{\lambda_l}{\delta}(T_{sl} - T_{lv}) = \dot{N}_{ev} m_{f,g} + h_v (T_{lv} - T_{sat}) \quad (6.3)$$

In the expression above, $h_v$ is a heat transfer coefficient introduced to characterise the process of sensible heat loss from the liquid surface to the bulk vapour. If we knew this vapour heat transfer coefficient, $h_v$, we could solve this for the intermediate liquid film temperature.
Knowing this, we can compute other quantities of interest. The rate of vapour generation is needed. From simple kinetic theory this is taken to be given by the difference between the rate of deposition of molecules onto the liquid surface, and the rate of emission from this surface. Emission is from a liquid surface at $T_{lw}$. Deposition is from a region of vapour at the system pressure $p_{sys}$ and a temperature of $T_{lw}$. All molecules that strike the liquid surface are assumed here to enter the liquid.

6.2.4 Net vapour generation rate

6.2.4.1 Preliminaries and basic kinetics results

It is helpful to gather a few basic kinetics results, available in various texts (Carey (1992)).

At a given temperature the (mean square) speed of the molecules is found from:

$$kT = \frac{m\bar{v}^2}{2} \quad (6.4)$$

or

$$\bar{v}^2 = \frac{2kT}{m} \quad (6.5)$$

The pressure due to collisions with the wall is

$$p = \frac{1}{3}N''''m\bar{v}^2 \quad (6.6)$$

so inserting the speed as a function of temperature, from (6.5) we have the pressure in terms of number density and temperature:

$$p = \frac{1}{3}N''''m\frac{2kT}{m} = \frac{2}{3}N''''kT \quad (6.7)$$

Similarly, the number density in terms of the pressure and temperature is:

$$N'''' = \frac{3}{2kT}p \quad (6.8)$$

The rate of collisions of vapour molecules, of number density $N''''$, and at temperature $T$ with the liquid film (‘wall collisions’) can be found via simple kinetic theory. Under the hypothesis
that the speeds of vapour molecules follow a Maxwell distribution, the rate of collisions with
the liquid surface is:

\[
\psi(T) = \frac{N''}{4} \sqrt{\frac{8kT}{\pi m}}
\]  

(6.9)

Substituting for the number density from (6.8) gives

\[
\psi(T) = \frac{p_s}{\sqrt{\frac{8kT_m}{\pi m}}}
\]  

(6.10)

### 6.2.4.2 Molecule deposition rate onto the liquid surface

By construction, we have a gas adjacent to the surface at a temperature \(T_{lv}\) and a pressure \(p_{sys}\). The rate of wall collisions, all here taken to be associated with deposition into the liquid, is then, from (6.10):

\[
\dot{N}_{dep}(T_{lv}) = \frac{p_s}{\sqrt{\frac{8kT_{lv}}{\pi m}}}
\]  

(6.11)

### 6.2.4.3 Molecule emission rate from a liquid surface

This is evaluated by asserting it to be equal to the deposition rate onto this surface from a vapour in equilibrium with such liquid; i.e., a vapour at \(T = T_{lv}\) and \(p = p_{sat}(T_{lv})\).

To estimate \(p_{sat}(T_{lv})\) use is made of Antoine’s equation (Antoine (1888)), an empirical fit for the vapour pressure, given for water via:

\[
p = \exp \left( A - \frac{B}{(C + T)} \right)
\]  

(6.12)

with constants in SI units:-

\[
A = 23.6363 \\
B = 4169.84 \\
C = -28.675
\]  

(6.13)

We use this in (6.11):

\[
\dot{N}_{em}(T_{lv}) = \exp \left( A - \frac{B}{(C + T_{lv})} \right) \sqrt{\frac{9}{8kT_{lv}\pi m}}
\]  

(6.14)
6.2.4.4 Net molecular evaporation rate

The net molecular emission, or evaporation, rate is found from the difference between emission and deposition rates, (6.14) and (6.11):

\[
\hat{N}''_{ev} = \exp \left( A - \frac{B}{(C + T_w)} \right) \sqrt{\frac{9}{8kT_w\pi m}} - P_{sys} \sqrt{\frac{9}{8kT_w\pi m}}
\]  

(6.15)

This tidies up to:

\[
\hat{N}''_{ev} = \sqrt{\frac{9}{8kT_w\pi m}} \left\{ \exp \left( A - \frac{B}{(C + T_w)} \right) - P_{sys} \right\}
\]  

(6.16).

6.2.5 Application of the model

We are now in principle able to solve (6.3), the heat balance, for the liquid – vapour interface temperature, making use of (6.16), via an iterative solution for \( T_w \). This is done using an arbitrary vapour heat transfer coefficient, and the various temperatures, heat fluxes and evaporation rates can thereby be evaluated for a range of values of vapour heat transfer coefficient. The numerical parameter values, and physical properties, used in the analysis are listed in Table 6-1.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity of the liquid</td>
<td>W m(^{-1}) K(^{-1})</td>
<td>0.679</td>
</tr>
<tr>
<td>Solid surface temperature</td>
<td>K</td>
<td>375.16 – 381.16</td>
</tr>
<tr>
<td>Vapour heat transfer coefficient</td>
<td>W m(^{2}) K(^{-1})</td>
<td>1 – 1,000</td>
</tr>
<tr>
<td>Film thickness</td>
<td>(\mu)m</td>
<td>0.1 - 10</td>
</tr>
<tr>
<td>Latent heat of evaporation</td>
<td>J Kg(^{-1})</td>
<td>2,260,000</td>
</tr>
<tr>
<td>Saturation temperature</td>
<td>K</td>
<td>373.16</td>
</tr>
</tbody>
</table>

Table 6-1: Physical properties and parameter values used in the model problem of liquid film evaporation explored.

6.2.6 The importance of sensible heat transfer

For even the highest value of vapour heat transfer coefficient considered, the very high value of 1,000 W m\(^{2}\) K\(^{-1}\), the sensible heat transferred to the vapour is tiny compared to that going to evaporate liquid. This is plain in Figure 6-6, where the evaporative and sensible heat fluxes
are plotted as a function of liquid film thickness, for three solid–liquid interface temperatures, 375.16, 377.16, and 381.16 K (i.e. superheats of 2, 4 and 8 K).

Figure 6-6: The evaporative heat flux and sensible heat flux for each of three film thickness, for wall superheats of 2, 4 and 8 K, as a function of film thickness, for a (high) vapour heat transfer coefficient of $10^3 \text{ W m}^{-2} \text{ K}^{-1}$.

The corresponding vapour ‘boundary layer’ temperature differences are shown in Figure 6-7.
It is useful to introduce an ‘evaporative heat transfer coefficient’, in order to quantify the relative importance of the resistance to the flow of heat (from the solid surface to the remote vapour) that is offered by the vaporization process. Tanasawa (1991) introduced a similar quantity in the context of condensation heat transfer. In that case, a temperature jump, occurring over a few molecular mean free paths, was postulated to exist between the liquid surface and the adjacent vapour. The heat transfer coefficient of phase change introduced by Tanasawa was defined as the constant of proportionality, \( h \), in the relationship between the latent heat flux of condensation (or, equivalently, evaporation) \( q'' \) and the temperature jump \( (T_{lv} - T_{vap}) \) between the liquid surface and the vapour immediately adjacent to it, \( q'' = h(T_{lv} - T_{vap}) \).

The approach adopted here is rather different, as no temperature jump is assumed at the liquid-vapour interface, and the temperature is taken to vary continuously, from its value at

Figure 6-7: Vapour ‘boundary layer’ temperature drop, for the three wall superheats considered, for each of three film thicknesses.
the liquid-vapour interface to its remote value. This variation is assumed to occur over a
distance much larger than a vapour molecular mean free path. A formal analogy to
convective heat transfer is introduced, and, in the continuum limit, the present equivalent
evaporative heat transfer coefficient is simply relating the heat flux at the liquid-vapour
interface to the temperature difference between that interface temperature and the saturation
temperature corresponding to the pressure prevailing in the body of vapour. In passing, we note how
this temperature variation, assumed to exist in the vapour, has very little effect on the rate of
deposition of molecules onto the liquid surface, and therefore on the evaporative heat flux, as
this is largely determined by the pressure in the vapour, which is a datum of our problem
and assumed to be set by external means, and much less by the vapour temperature.

As explained in the preceding text, it is actually a pressure difference between the emitted and
impinging fluxes of vapour that drives the evaporation, while in the definition of the
evaporative heat transfer coefficient a temperature difference is involved. This notion of
evaporative heat transfer coefficient hence has to be regarded as a practical means of
incorporating, into continuum mechanics descriptions of boiling heat transfer, a finite
reluctance of the evaporative flow of heat - as opposed to the usual treatment that assumes
zero reluctance.

Not plotted (it adds nothing), the effective evaporative heat transfer coefficient can be
extracted for all these cases (of different film thicknesses, and three different superheats). This
is here computed as:

$$h_{ev} = \frac{1}{T_{sl} - T_{sat}(p) - \frac{\delta}{\lambda}} - h_{v} \quad (6.17)$$

where $q_{tor}^\eta$ is the sum of sensible and latent heat fluxes. For all cases the value is $1.17 \times 10^7 \text{ W m}^{-2} \text{ K}^{-1}$. This is many times any credible vapour heat transfer coefficient. It is safe to conclude
that the mechanism suggested in Bornhorst and Hatsopoulos (1967), of the evaporative
process being materially influenced by the liquid – vapour interface being above the
saturation temperature, is not significant under the conditions of these observations.
6.2.7 Simplified evaporative heat transfer coefficient

With the sensible heat transfer confirmed as negligible, we can make a rather simpler estimate of the evaporative heat transfer coefficient. We introduce a superheat defined via

\[ T_{\text{sup}} \equiv T_{lv} - T_{\text{sat}} \]

The rate of molecular deposition onto the surface is, from (6.11):

\[ \dot{N}_{\text{dep}}(T_{\text{sup}}) = p_{\text{sys}} \sqrt{\frac{9}{8k(T_{\text{sat}} + T_{\text{sup}})\pi m}} \]  

(6.18).

The rate of emission is, from (6.14):

\[ \dot{N}_{\text{em}}(T_{\text{sup}}) = \exp\left( A - \frac{B}{C + (T_{\text{sat}} + T_{\text{sup}})} \right) \sqrt{\frac{9}{8k(T_{\text{sat}} + T_{\text{sup}})\pi m}} \]  

(6.19)

and the net rate of evaporation is thus:

\[ \dot{N}_{\text{ev}}(T_{\text{sup}}) = \frac{9}{\sqrt{8k(T_{\text{sat}} + T_{\text{sup}})\pi m}} \left\{ \exp\left( A - \frac{B}{C + (T_{\text{sat}} + T_{\text{sup}})} \right) - p_{\text{sys}} \right\} \]  

(6.20)

and, expressed as a heat flux:

\[ \dot{q}_{\text{ev}}(T_{\text{sup}}) = m h_f \sqrt{\frac{9}{8k(T_{\text{sat}} + T_{\text{sup}})\pi m}} \left\{ \exp\left( A - \frac{B}{C + (T_{\text{sat}} + T_{\text{sup}})} \right) - p_{\text{sys}} \right\} \]  

(6.21).

If this evaporation rate is plotted against the liquid surface superheat it is seen to be close to linear. The ratio of heat flux to superheat gives the effective heat transfer coefficient for evaporation, based on this simple kinetic theory, and this is plotted for a range of surface superheats in Figure 6-8, and from which the limiting value as equilibrium (zero surface superheat) is approached, can be extracted. As would be expected, it is the \(1.17 \times 10^7\) W m\(^{-2}\) K\(^{-1}\) noted above.
Figure 6-8: Evaporative heat transfer coefficient as a function of the superheat of the liquid surface.

6.2.8 Conclusions from this simple kinetics analysis

Sensible heat transfer, causing the local vapour to be hotter than the remote, is not influencing the system. Broadly, the thermal resistance of the evaporative process as inferred from this analysis will equal that of the conduction through the liquid for a film thickness of ~0.06 microns. For a one-micron film the thermal resistance of the evaporative process will be ~1/20 of the conductive resistance. This is too little an effect to resolve the anomaly noted. This simple kinetics model, with all impinging molecules assumed to enter the liquid, thus does not explain the observations.

6.3 The ‘imperfect condensation’, or ‘partial stick’ approach

6.3.1 The basis of the model

This approach, originally developed by Schrage (1953), is described several review works, notably that of Marek and Straub (2001), and Eames, Marr et al. (1997). Here a condensed summary of its essentials is presented.
As in the ‘simple kinetics’ analysis above, in equilibrium conditions (no net mass transfer across the interface), the flux of molecules emitted from the surface and the flux of molecules impinging on the surface are equal. As was done above, it is possible to evaluate the equilibrium impinging flux, given the pressure and temperature of the gas in contact with the liquid. Having done so, the rate of emission of molecules from the liquid surface at equilibrium is also determined, as being, by construction, equal to this impingement rate. The straightforward algebra of this is given above.

However, this is predicated on the rate of wall collisions predicted from the simple kinetic theory being one and the same as the rate at which vapour molecules enter the liquid phase; i.e., all incident molecules ‘stick’. As explained by Schrage, it is probable that only a fraction of incident molecules stick to the liquid surface, other are reflected. Various terminology is used (Carey (1992)), and additional complexities are required in particular in the case (not relevant here) of multi-species systems, with further complexity introduced in the form of considerations of ‘reflection back’ of escaping liquid molecules. However, as observed above, the observed rate of evaporation of liquid molecules is grossly less than the rate at which vapour molecules strike the liquid surface, implying that the fraction that sticks of those that strike must be well below one.

### 6.3.2 Model formulation

The starting point is (6.3), with the sensible heat transfer ignored, and as above, $T_{sup}$ the degree to which the liquid surface is above saturation:

$$\frac{\lambda_l}{\delta} (T_{sl} - T_l) = N_{ev}'' m_{fg}$$  \hspace{1cm} (6.22)

Net evaporation is found via (6.20) with the deposition and hence evaporation rates both reduced by a factor (here, $f$) to reflect only partial ‘sticking’, giving a net evaporation rate of

$$N_{ev}'(T_{sup}) = f \sqrt{\frac{9}{8kT_l \pi m}} \left\{ \exp \left( A - \frac{B}{(C + T_l)} \right) - P_{sat} \right\}$$  \hspace{1cm} (6.23)

and combining these we have:
\[
\frac{\lambda}{\delta} (T_s - T_w) = m h_{fs} f \sqrt{\frac{9}{8kT_{fs} \pi m}} \left\{ \exp \left( A - \frac{B}{(C + T_w)} \right) - p_{sat} \right\}
\] (6.24).

As before, we can solve this numerically for \( T_w \), and then compute other quantities of interest.

As an illustrative example, Figure 6-9 shows the variation of heat flux with film thickness for a typical wall superheat. The importance of the partial sticking is evident.

Figure 6-9: Effect of partial sticking of impinging molecules on film evaporation.

6.3.3 Application to the Jung & Kim cases

It is attempted to determine this sticking fraction by examination of the Jung and Kim results.

In the next section we will extract measurements of the heat flux, which obviously in the experiments vary with both solid-liquid interface temperature, and with the film thickness. Predictions of heat flux for these cases will be made using the simple kinetics model, modified by various sticking fractions.

In the following section we will extract from the experiments an effective evaporative heat transfer coefficient, and then use the simple kinetics model to predict an evaporative heat transfer coefficient as a function of the sticking fraction.
6.3.3.1 Inferring of sticking fraction via the heat flux

In Figure 6-10 we plot the heat fluxes measured directly (‘optical’ and ‘finite element’) by Jung and Kim, and the heat flux they inferred derived from the perfect evaporation model. Alongside these we plot the heat flux predicted by the simple kinetics model above, and by this simple kinetics model modified to take into account ‘imperfect sticking’.

![Graph showing heat flux vs. film thickness](image)

Figure 6-10: Application of the evaporation model that includes partial sticking of impinging molecules to the Jung & Kim data set.

This provides good evidence that a sticking fraction between 0.10 and 0.01 is required in order restore consistency between the modelled film evaporation rate and the two independent, mutually consistent measurements.

6.3.3.2 Inferring of sticking fraction via the evaporative heat transfer coefficient

As discussed earlier, the value of evaporative heat transfer coefficient is here inferred from the two independent heat flux assessments, and from the film thickness and wall temperature measurements.
As justified by the previous analysis, the sensible flow of heat from liquid film to vapour is neglected, i.e. the latent enthalpy flow (at the liquid vapour interface) is assumed equal to the sensible enthalpy flow at the solid-liquid interface, driven by the temperature difference between its upper and lower surfaces. The energy balance of the film can be written as:

$$\frac{\lambda}{\delta}(T_u - T_v) = \dot{q}''$$

(6.25)

or

$$\frac{\lambda}{\delta} \left[ (T_{sat} - T_{SAT}) - (T_u - T_{SAT}) \right] = \dot{q}''$$

(6.26).

Combining this and the equation (6.17), and neglecting $h_v$, one can write:

$$\frac{\dot{q}''}{T_{sat} - T_{SAT}} = h_{TOT} = \frac{1}{\delta \lambda + \frac{1}{h_{ev}}}$$

(6.27).

The quantity $h_{TOT}$ is a global heat transfer coefficient, including the conductive thermal resistance of the film and the evaporative resistance. The heat flux, film thickness and solid-liquid interface temperature are known from measurements, which allows the relating $h_{TOT}$ to the film thickness. The as yet unknown evaporative heat transfer coefficient can be inferred fitting a line through the experimental points, as shown in Figure 6-11. As the film thickness $\delta$ goes to zero, so does the conductive resistance, and the global heat transfer coefficient tends to the evaporative heat transfer coefficient. We can thus take the value at the origin as indicative of the evaporative htc. The value so obtained is approximately 240 kW/m²/K.
Figure 6-11: Best fit of the global heat transfer coefficient of an evaporating liquid film, inferred from independent measurements of the heat flux associated to microlayer evaporation, and from optical measurements of the film thickness.

Using the approach outlined in Section 6.3 above, we can determine the variation of the effective evaporative heat transfer coefficient with the sticking fraction. The results of doing so are plotted in Figure 6-12.
Figure 6-12: Variation of equivalent evaporative heat transfer coefficient for different values of sticking fraction.

We see that the value of about 240 kW/m²/K implicit in the Jung and Kim results, obtained above, is obtained with a sticking fraction of approximately 0.02.

6.4 Approach based on Boltzmann Transport Equation

6.4.1 The basis of the model

In recent years an alternative to the simple kinetic theory approach has been proposed for calculating the temperature and pressure at the interface during evaporation and condensation ((Pao 1971), (Pao 1971)). This alternative approach uses a linearized form of the Boltzmann Transport equation (Boltzmann-Krook-Welander or BKW equation) in the vapour close to the interface to calculate the local variation in temperature and density. A detailed application of this approach is provided by Sone and Onishi who derived numerical values for the temperature and pressure jump at the interface between a condensed phase and its vapour assuming: (i) that deviations from equilibrium conditions are small, (ii) that the gas molecules leaving the surface of the condensed phase have a Maxwell velocity distribution corresponding to saturation conditions at the surface temperature of the condensed phase, and (iii) that that all incident vapour molecules are condensed at the phase boundary (complete condensation/evaporation condition). These workers came to the conclusion that a temperature jump would exist at the interface even in the continuum limit in which the mean
free path of the vapour molecules becomes vanishingly small. Their equation for the temperature jump can be expressed as:

\[ T_{\text{remote}} = T_w \left( 1 - \zeta_T \frac{v}{\sqrt{2RT_w}} \right) \]  \hspace{1cm} (6.28)

where \( \zeta_T \) is a temperature jump coefficient, \( T_w \) is the temperature of the condensed phase at the interface, \( T_{\text{remote}} \) is the bulk vapour temperature away from the interface, and \( v \) is the bulk net vapour velocity due to evaporation or condensation. The analysis gave the temperature jump coefficient as \( \zeta_T = 0.447 \) independent of vapour species and its temperature.

Using the fact that \( q_{ev}'' = u_p h_{fg} \), an equivalent evaporative heat transfer coefficient, defined via \( q_{ev}'' = h_e (T_w - T_{\text{remote}}) \) can be obtained. Assuming the bulk vapour temperature \( T_{\text{remote}} \) is the saturation temperature \( T_{\text{SAT}} \) defined in the preceding text, it follows from (6.28), with \( \zeta_T = 0.447 \):

\[ h_e = \frac{2.24 \rho h_{fg} \sqrt{2R}}{T_{\text{SAT}}^{1/2}} \]  \hspace{1cm} (6.29)

This is notably different from the form derived from simple kinetic theory, but analogous to the evaporative heat transfer coefficient of Schrage, introduced in the previous chapter. However, for water evaporating into its vapour at atmospheric pressure, equation (6.29) gives a value of 8.4 MW m\(^{-2}\) K\(^{-1}\), which is reasonably consistent with the 1.17x10\(^7\) W m\(^{-2}\) K\(^{-1}\) of the simple kinetics model evaluated for the case of perfect condensation.

**6.4.2 Comparison with the Jung & Kim results**

In Figure 6-13 the predicted global heat transfer coefficient \( h_{\text{TOT}} \), calculated using an evaporative heat transfer coefficient obtained from the BKW approach, (6.29), is plotted against film thickness. The experimental results of Jung and Kim are also shown. Shown for comparison are the predicted values of evaporative htc obtained by assuming thermal equilibrium at the vapour-liquid interface (taking the interface at the saturation temperature), which are little different from those obtained using the BKW model. As concluded earlier
above, the discrepancy seems likely to be a result of the assumption that all incident molecules enter the liquid. Following an approach essentially identical to that employed in the section above, it turns out that a sticking fraction of approximately 0.03 is required to establish broad consistency between the experimentally derived heat transfer coefficient, and that predicted by the BKW model.

![Comparison of BKW model with data](image)

**Figure 6-13**: Comparison of prediction of the total heat transfer coefficient of the liquid film from Boltzmann-Krook-Welander analysis with experimental data of Figure 6-11.

6.5 Discussion

6.5.1 Conclusions of the present analysis

The simple kinetics analysis confirms that sensible heat flows in the vapour, suggested by Bornhorst and Hatsopoulos (1967) and others to be significant, are not important, at least under the present conditions.

The evaporation rate, or equivalently effective evaporative heat transfer coefficient, that simple kinetics predicts is similar to that predicted by the more sophisticated BKW model, and both are grossly too high to fit the results.
The present conclusions are in broad agreement with earlier suggestions. Experiments by Adera, Antao et al. (2016) of thin film evaporation at low pressure (3 kPa) in a wick evaporator suggest a sticking fraction of about 0.07. Carey (1992) recommends values of \( f \) close to 0.03 – 0.04, based on a survey of experimental works. Under the circumstances of these measurements, the effective evaporative heat transfer deduced from the present measurements is not inconsistent with the value of 770 kW/m\(^2\)/K deduced, for water at atmospheric pressure, by Yabuki and Nakabeppu (2016).

In essence, experiments discussed here indicate that the inclusion of imperfect condensation - that only a fraction of molecules incident on the liquid surface actually enter the liquid - provides a plausible explanation of the behaviour, with a ‘stick fraction’ in the range 0.02 – 0.07. As such, the experiments actually provide a relatively well-characterised opportunity for the evaluation of this quantity, embodying as they do a less uncertain liquid surface temperature than is commonly the case.

### 6.5.2 Implications of the partial sticking hypothesis

The analysis here presented suggests that only a small fraction, approximately 1/30, of incident vapour molecules is absorbed by the upper surface of the liquid film during microlayer evaporation. In principle, this is expected to occur whenever liquid is evaporating from a surface exposed to saturated vapour. We now explore the implications of this empirical observation in the context of elementary molecular dynamics, in particular as regards modelling of molecular forces within fluids.

It is useful to identify first a possible relationship between sticking fraction and molecular speed distribution of vapour molecules.

Under the assumption that the speeds of vapour molecules follow the Maxwell distribution, the fraction of molecules with speed smaller than a certain threshold value (cumulative speed distribution) is shown in Figure 6-14. Also shown is the most probable speed.

The graph suggests that it is possible to use appropriate threshold values of the molecular speed to identify the sticking fraction.
Fig. 6-14: Cumulative Maxwellian distribution of molecular speeds in an ideal gas.

It is reasonable to formulate the hypothesis that only molecules with a speed below a certain threshold value stick to the surface. This can be thought of as consequence of the nature of the forces between molecules, which are believed to be repulsive at very short range, and attractive at a longer range (Carey (1992)). The nature of these forces, which are subject to considerable speculation, matters little for present purposes; however, to get a sense of scales, both forces decline over length scales that are much shorter than the range of influence of the familiar Coulomb interaction (proportional to the reciprocal of the distance between charged particles). These intermolecular forces are usually described as originating from a potential field, generated in the surrounding space by each molecule. As described by models like that of the Lennard-Jones potential, shown in (Figure 6-15), the combination of the two opposing fields results in a potential well. The depth of the well is the minimum energy that needs to be provided to a molecule in close proximity to another in order to bring it at an arbitrarily large distance.
Figure 6-15: Qualitative illustration of the Lennard-Jones potential of interaction between molecules in a fluid. Adapted from Carey (1992).

After the (elastic) collision with the surface layer of liquid molecules, a vapour molecule with moderate velocity will not have enough energy to escape, and will be ‘absorbed’ by the layer. On the other hand, sufficiently energetic molecules will bounce off. Using plausible values for the energy $E$ associated to the potential well, the corresponding molecular speeds are shown in Figure 6-16. These threshold speeds correspond to a certain fraction of molecules, those with speeds not exceeding the value, which are therefore absorbed.
Figure 6-16: Significant values of the maximum speed of molecules following a Maxwellian distribution that stick to the surface, under the hypothesis that only the impinging molecules with speed below a given threshold stick to the liquid surface.

To get a sense of scales, the threshold speed corresponding to a fraction of absorbed molecules of 0.03 is approximately 47 m/s, or 1/3 of the most probable speed of the Maxwell distribution (~138 m/s). On the other hand, almost perfect sticking (90% of impinging molecules get absorbed) occurs for an $E$ value of $10^{-21}$ J, corresponding to roughly two times the most probable speed.

The implication of these speculations is that the fraction of incident molecules that stick to the surface, and therefore the evaporation rate and equivalent heat transfer coefficient, depend on the energy value $E$ of the Lennard-Jones model, or similar models (Mark and Nilsson (2001), Berendsen, Grigera et al. (1987)). Considerable uncertainty surrounds plausible values of this quantity, likely in the range $10^{-22} - 10^{-20}$ J.

It is understood that large variations in values of evaporative heat flux and heat transfer coefficient are induced by variations of the $E$ value, as shown in Figure 6-17.
Figure 6-17: Evaporation rate from a liquid surface exposed to its vapour, and equivalent evaporative heat transfer coefficient, for different values of the Lennard-Jones potential well depth (E value).

What matters here is that E values, around $10^{-21}$ J, corresponding to the empirical sticking fraction of approximately 0.03 here recommended, are not excluded by commonly accepted estimates of this difficult parameter of molecular interaction models.
CHAPTER 7
EFFECT OF EVAPORATIVE THERMAL RESISTANCE ON MODELLED STEAM BUBBLE GROWTH

This chapter describes the incorporation of evaporative heat transfer in the microlayer sub-grid model of the PSI-BOIL code. The microlayer model here adopted, and its augmentation to include an evaporative heat transfer coefficient, are described. The influence of evaporative resistance on computed steam bubble development at atmospheric pressure is explored. Comparison with recent measurements is discussed, showing good agreement and suggesting directions for future work.

7.1 Incorporation of evaporative thermal resistance in the PSI-BOIL microlayer sub-grid model

The microlayer sub-grid model of the ITM code PSI-BOIL, described in Chapter 3, has been augmented to include ‘imperfect’ evaporation. The treatment of Tanasawa, described in Chapter 5, and the notion of an evaporative heat transfer coefficient, are here adopted.

An evaporative thermal resistance, as defined in Chapter 3, is introduced to model heat transfer from the upper microlayer surface to the vapour.

Figure 7-1: Inclusion of evaporative heat transfer in the microlayer depletion model.
Note that in Figure 7-1 we have shown an indicative ‘step’ in temperature at the liquid-vapour interface, associated with the interface thermal resistance under investigation. The local evaporative heat flux is now computed as:

\[
\dot{q}_{\text{vl}}'' = \frac{T_s - T_{\text{SLT}}}{\delta + \frac{1}{\lambda} + h_{ev}}
\]  

(7.1).

The evaporative heat transfer coefficient \(h_{ev}\) is an additional free parameter. In the analysis presented in chapter 4, a plausible value has been inferred, of ~240,000 W/m\(^2\)/K, and will be adopted here. Plainly, for fluids other than water, and at pressures other than atmospheric, the value is expected to be different.

The sub-grid microlayer sub-grid model is used to update the volumetric mass source and heat sink terms, localised at the bubble base according to the sketch shown in Figure 7-2, where an indicative CFD grid has been drawn (the algebraic model is not active in the dry patch, the ‘dry cells’ of the figure). Based on the cell-wise values of the mass source, the volumetric evaporation heat sink required for conjugate heat transfer is updated. Using these new sink and source terms, the color function and temperature fields are updated, and the algebraic microlayer computation is applied again to the updated configuration of bubble base.

Figure 7-2: Finite volume representation of microlayer depletion.
Computation of microlayer depletion is carried out explicitly, using the solid temperature and microlayer thickness at time $n$ in order to compute the temperature and heat flux at the solid-liquid interface at time $n+1$.

The full advancement procedure of the microlayer depletion computation is coupled to the interface tracking method described in chapter 3, as follows:

1) Compute evaporation at the bubble curved surface;
2) Compute $T_{sl}$ from the energy balance at the solid-liquid interface:

$$
\lambda \left( \frac{T_s - T_{sl}}{dz/2} \right) = \frac{T_s - T_{SAT}}{\delta^n + \frac{1}{\lambda_l h_{ev}}} \quad (7.2)
$$

3) Compute the heat flux:

$$
q_{ml}'' = \frac{T_s - T_{SAT}}{\delta^n + \frac{1}{\lambda_l h_{ev}}} \quad (7.3)
$$

4) Compute microlayer depletion:

$$
\delta^{n+1} = \delta^n - \frac{1}{\rho_l h_{fs}} \frac{q_{ml}''}{\Delta t} \quad (7.4)
$$

5) Compute microlayer evaporation rate and heat sink, based on microlayer depletion, and communicate values to the interface tracking computation;

6) Compute the body force;
7) Update velocity and pressure;
8) Update color function;
9) Update temperature;
10) Go back to 1).
7.2 The model problem

7.2.1 Physical model of steam bubble development

We consider bubble growth at a horizontal heated surface, bounding an extended pool of saturated water (Figure 7-3), at atmospheric pressure. The physical model includes conjugate heat transfer with a substrate of finite thermal diffusivity.

As an initial condition, the solid is at a uniform temperature, $T_\infty$. The near-wall liquid is superheated, its temperature decreasing with the vertical distance from the heat transfer surface, until the saturation value $T_{SAT}$ is reached. The overall superheat available for bubble expansion is the temperature difference $\Delta T = T_\infty - T_{SAT}$. The bubble grows due to the addition of heat from the superheated liquid and from the substrate. Bubble development is simulated for 10 ms, a time typical of the diffusion-controlled growth of isolated bubbles during nucleate boiling of atmospheric water in laboratory conditions. Simulations are repeated for three cases with varying driving temperature difference, $\Delta T =$5, 10, and 15 K.

Figure 7-3: Physical model of steam bubble development in conditions for which microlayer evaporation is an important contribution to bubble growth. Showing inclusion of conjugate heat transfer with the substrate in the ITM model, and an indicative initial variation of the temperature long the vertical direction.
7.2.2 Exploratory analyses

Before running the proper hydrodynamic and thermal model, the thermal response of the solid to microlayer evaporation has been investigated with simple finite difference and finite volume representations of the unsteady temperature distribution in the substrate.

7.2.2.1 1D model

The system solid substrate – evaporating water film – vapour is considered. In Figure 7-4, the expected vertical temperature distribution in the solid and in a depleting liquid film of thickness $\delta$, assumed to extend to infinity in the other two spatial directions, is sketched. Indicative temperature drops in the solid ($T_\infty - T_{sl}$), in the film ($T_{sl} - T_{lv}$) and at the liquid-vapour interface ($T_{lv} - T_{SAT}$) are drawn at two times into the computation, showing depletion of the film and relaxation of the temperature profile in the solid.

![Diagram](image)

Figure 7-4: One-dimensional model of the system solid-film-vapour used to model microlayer depletion.

In the proposed thermal model, the vapour phase is taken to be at the saturation temperature at atmospheric pressure. Evaporative thermal resistance at the liquid-vapour interface is modelled as discussed in the preceding text. The liquid film initial thickness is a free parameter. For computations shown here, the film is set to be initially two microns thick. The solid is treated as a semi-infinite thermal conductor. The liquid film and the solid are initially
at a uniform temperature $T_\infty$, higher than the saturation temperature. The total available temperature difference driving evaporation is $\Delta T = T_\infty - T_{SAT}$.

The computational domain consists of a finite depth of solid, equal to several times the penetration depth into the solid computed based on the typical time scale of full microlayer depletion (a few milliseconds, given the initial film thickness here considered). This allows fixing the temperature at the bottom boundary of the solid domain, to a value equal to $T_\infty$.

The unsteady temperature distribution in the solid is advanced with an explicit finite difference method. Film depletion due to evaporation is computed assuming a thermally thin film and continuity of the heat flux at the solid-liquid and liquid-vapour interfaces. The evaporated film thickness per unit time is therefore proportional to the temperature difference between the lower and upper surface of the film, divided by its thickness. The rate of depletion of the film corresponds to a time dependent heat flux, applied as an explicit time-dependent Neumann boundary condition of the one-dimensional Fourier equation solved in the solid.

The numerical procedure used to advance the temperature distribution in the solid was benchmarked against the analytical solution by Carlslaw and Jaeger (1959) for the 1D Fourier equation for a semi-infinite conductor with a Robin boundary condition representing convective heat transfer. A time step of $0.05 \frac{\Delta x^2}{a_s}$ was required to obtain satisfactory agreement between the mesh converged boundary heat flux, and that computed from the analytical solution, Figure 7-5.
Besides the mesh sensitivity study, a preliminary analysis was conducted in order to elucidate the influence of thermal conductivity of the solid on film depletion, for the case of a typical \((T_{\infty} - T_{sat})\) value of 10 K. At equal heat capacity, the thermal conductivity has been varied as a free parameter within the range 10-70 W/m/K. The importance of this material property as regards film depletion is clear, as shown in Figure 7-6, where the evaporation heat flux corresponding to microlayer depletion is seen to depend on the thermal conductivity value.
The case of thermal conductivity of 50 W/m/K and 10 K of driving temperature difference was then considered. Evaporative resistance is set equal to \(4.1 \times 10^{-6}\) W/m²/K, representative of the values deduced in the analysis presented in the previous two chapters. Inclusion of evaporative heat transfer decreases significantly the microlayer depletion rate, if compared to the case whereby the upper film surface is taken at the saturation temperature, Figure 7-7. In this 1D model, the total liquid mass per unit area of film that can evaporate is equivalent to the initial film thickness; therefore the same overall evaporated mass is computed at the end of the simulated transient (full depletion of the film), Figure 7-8, being the initial film thickness the same in the two cases considered.
Figure 7-7: Computed microlayer evaporation rate from 1D transient conduction model, with and without evaporative resistance.

Figure 7-8: Total mass fluence from microlayer depletion, with and without evaporative resistance.

It is worth evaluating the relative importance of the resistances to the flow of heat here considered. Continuity of the heat flux at the solid-liquid and liquid-vapour interfaces requires that

\[ q''_{lv} = \frac{T_{\infty} - T_{SAT}}{P_s + P_l + P_{lv}} \]  

(7.5).
The temperature $T_{lv}$ of the liquid surface is computed, given the (constant) evaporative heat transfer coefficient and the instantaneous heat flux. The time-dependent film thickness is similarly given by the numerical procedure. It is thus possible to compute the thermal resistances involved in the evaporation process as follows:

$$P_{ev} = \frac{T_{lv} - T_{SAT}}{\dot{q}_{ev}}$$

$$P_f = \frac{\delta}{\lambda}$$

$$P_s = \frac{T_{\infty} - \bar{T}_{SAT}}{\dot{q}_{ev}''} \left( \frac{\delta}{\lambda} + \frac{1}{h_{ev}} \right)$$

(7.6).

By construction, evaporative resistance is constant, and the liquid conductive resistance declines with time, due to film depletion, Figure 7-9. Interestingly, evaporative resistance appears at all times to be at least comparable to the resistance in the solid.

![Figure 7-9: Temporal variation of the series of thermal resistances of the solid, of the film of the evaporation process offered by the system solid-microlayer-interface.](image)

7.2.2.2 2D axisymmetric model

The unsteady temperature distribution in the solid is solved with an axisymmetric, explicit in time, finite volume model (Versteeg and Malalasekera (2007)). Given the initial microlayer
geometry - taken from the measurements -, the film depletion equations (7.3) and (7.4) are implemented as a time dependent, explicit in space, Neumann boundary condition, Figure 7-10. At locations where the film thickness decreases below the arbitrary value of 0.1 nm, a dry-out condition is imposed, namely thermal insulation of the solid boundary.

![Diagram](image)

**Figure 7-10:** Two-dimensional, axisymmetric transient conduction model of the thermal response of the solid to microlayer evaporation. For comparison with experimental data of Jung, Chung et al. (2015), the properties of calcium fluoride have been used in the computation.

The conditions of the simulation reproduce the boiling of water at atmospheric pressure performed by Jung, Chung et al. (2015), already discussed. The computational domain is a cylinder of radius \( R = 2000 \) microns and height \( H = 1000 \) microns. All boundaries are adiabatic except the top face in contact with the microlayer, where the boundary condition described in the preceding text is applied. A uniform temperature equal to 117°C is adopted as an initial condition in the solid domain.

For comparison with the experimental data, the thermophysical properties of calcium fluoride have been chosen to model the unsteady temperature distribution in the substrate.

The density value is approximately constant far from phase transition points. Low values of thermal expansion coefficient are reported in the literature (Corning-Inc. (2003)), therefore the density is taken equal to the value at room (25 °C) temperature of 3180.0 kg/m³.

According to vendors (Corning-Inc. (2003)), the thermal conductivity and specific heat capacity are expected to exhibit a dependency on temperature. Variations in thermal...
conductivity are large between approximately 100 and 300 °C, Figure 7-11. However, within the narrow range of temperatures here considered (17 °C at most), the thermal conductivity of calcium fluoride does not vary significantly. Therefore, the value at 100°C, judged to be of 54.0 W/m/K, has been chosen for the rest of the analysis.

![Thermal conductivity graph](image1.png)

Figure 7-11: Thermal conductivity of commercial calcium fluoride as a function of relative temperature.

No data on the specific heat capacity was found at the temperatures of interest here. Based on available information about the dependency on temperature of the specific heat of calcium fluoride, Figure 7-12, an extrapolation was performed in order to estimate the value of specific heat at 373.16 K, judged equal to 862.0 J/Kg/K.

![Specific heat capacity graph](image2.png)

Figure 7-12: Specific heat capacity of commercial calcium fluoride as a function of absolute temperature.
Mesh sensitivity of the numerical procedure was assessed testing four different levels of uniform discretisation, corresponding to cell sizes of 3.9, 7.8, 15.6 and 31.2 microns. Time steps equal to $0.05 \frac{\Delta x^2}{\Delta t}$ have been used. The time-dependent spatially-averaged evaporation rate of the liquid film as a function of time is shown in Figure 7-13 for different levels of discretization. Convergent behaviour is observed.

The radial distribution of the heat flux at the solid-liquid interface is shown in Figure 7-14 at various times after bubble nucleation – 1, 4 and 7 ms - that are representative of the early stages of bubble development.

![Figure 7-13: Mesh sensitivity of the thermal model of the solid substrate.](image-url)
Figure 7-14: Microlayer depletion rate, for various evaporation coefficients, computed with a two-dimensional axisymmetric transient conduction model of the boiling substrate, compared to experimental data by Jung, Chung et al. (2015).
Results are shown for various evaporation coefficients, namely 1.00, 0.10 and 0.01. At all times considered, the effect of incorporating the evaporative resistance is most evident near the dry patch, where microlayer is the thinnest. For small microlayer thicknesses the fraction of the total (conductive plus evaporative) resistance to the flow of heat offered by the evaporative mechanism is of course the largest. To get a sense of scales, in the present conditions, at seven milliseconds after bubble nucleation, the evaporative resistance corresponding to an evaporation coefficient equal to 0.1 is about seven times the conductive resistance offered by the smallest thickness (adjacent to the dry patch) of microlayer measured by Jung. At all instants of time, a reduction of the evaporation coefficient – and hence an increase in evaporative resistance – is accompanied by a reduction of the computed boundary heat flux, and in a slowing of the growth of the dry area created by microlayer retreat. Both effects are independent of the ‘macroscopic’ hydrodynamics and heat transfer of bubble growth, which are not part of the present analysis. Most importantly, a marked spike in the computed heat flux distribution observed near the dry patch for the largest evaporation coefficient ($f = 1.00$) is considerably reduced as the evaporation coefficient is reduced, and the resulting radial distribution of the heat flux appears flattened out. At each time, the values of measured heat flux at different radial locations (corresponding to very different microlayer thicknesses) are similar (to get a sense of scales, the maximum microlayer thickness is around 5 microns, while for a significant radial extent the microlayer thickness is below 0.5 microns). This flat distribution of the computed heat flux is in good qualitative agreement with the measurements.

**7.2.3 CFD model of steam bubble development**

Exploiting symmetry, a quarter of the physical domain is simulated, Figure 7-15. The thickness of substrate included in the domain is several times the thermal penetration depth $\delta_{th}$ computed based on the simulated time $t_{sim}$, $\delta_{th} = \sqrt{t_{sim} \lambda / \rho c_p}$. Effects of the boundary condition applied at the bottom of the domain are thereby nullified.

The vertical planes opposite the two symmetry planes are impermeable and adiabatic; flow of heat and mass is allowed only through the top boundary of the domain, where a remote liquid temperature is specified (equal to the saturation value $T_{SAT}$).
Figure 7-15: Computational domain of the ITM model of steam bubble development in conditions for which microlayer evaporation is significant to bubble formation. A single steam bubble nucleating on a calcium fluoride substrate in atmospheric conditions is considered.

The size of the domain was chosen by trial and error in order to minimise the influence of boundary conditions on computed bubble development. The domain is uniformly discretized in the region where the bubble develops; outside this volume use is made of mesh stretching in order to limit the computational cost.

As an initial condition, a seed of vapour, of radius equal to one cell, is placed on the heat transfer surface at the intersection of the two planes of symmetry. The seed rapidly grows to be much larger than its initial size. The initial vertical spatial variation of temperature in the liquid is set assuming a transient conduction process, according to the following expression:

\[
T(z) = T_{\text{SAT}} + (T_\infty - T_{\text{SAT}}) \text{erfc} \left( \frac{z}{2 \sqrt{\Delta t_{\text{preheat}} \alpha}} \right)
\]  

(7.7)

where \( \Delta t_{\text{preheat}} = 10 \, \text{s} \), adjusted with a trial and error procedure in order to obtain an initial superheated liquid layer of approximately 1.5 millimetres, not untypical of observed thermal boundary layers (Kim (2016), Yabuki, Hamaguchi et al. (2012)).
The microlayer geometrical parameters $C$ and $\gamma$ are respectively set equal to 0.00446 and 1, based on experimental evidence by Utaka, Kashiwabara et al. (2013).

### 7.2.4 Mesh sensitivity study

The computational domain is uniformly discretized in the space where the bubble develops. Outside this region, where details of the flow field less unimportant, the mesh has been stretched in order to limit the time to run the computations. Mesh sensitivity of the model has been assessed with four different levels of discretization, shown in Table 7-1. The symbol $\Delta x_p$ refers to the side of the cubes into which the region where the bubble develops has been discretised; $\Delta z_s$ is the vertical dimension of a solid cell.

<table>
<thead>
<tr>
<th>Mesh n.</th>
<th>$\Delta x_{min}$ [µm]</th>
<th>$\Delta z_s$ [µm]</th>
<th>NXxNYxNZ</th>
<th>n. cells</th>
</tr>
</thead>
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<td>166.66</td>
<td>28x28x56</td>
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</tr>
<tr>
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<td>83.33</td>
<td>83.33</td>
<td>52x52x104</td>
<td>281,216</td>
</tr>
<tr>
<td>3</td>
<td>41.67</td>
<td>41.67</td>
<td>100x100x200</td>
<td>2,000,000</td>
</tr>
<tr>
<td>4</td>
<td>20.83</td>
<td>20.83</td>
<td>196x196x480</td>
<td>18,439,680</td>
</tr>
</tbody>
</table>

Table 7-1: Parameters of mesh sensitivity study of the ITM model of steam bubble development in conditions for which microlayer evaporation is significant as regards bubble formation.

The mesh sensitivity study has been performed for the case of $T_\infty - T_{SAT} = 10$ K, and taking the upper surface of the microlayer at the saturation temperature. As in the computations that follow, the equilibrium contact angle is set equal to 60°. Time histories of equivalent bubble diameter are plotted in Figure 7-16 for different meshes, showing a dependency on discretization of the computed bubble size. As seen in Figure 7-17, showing the equivalent bubble radius after 8 ms into the simulation, if the number of cells along a given direction is doubled (a uniform discretization has been used), a variation in bubble size of approximately 15% is observed.
Figure 7-16: Time history of equivalent bubble diameter for different levels of mesh refinement. The case of a single steam bubble nucleating on a calcium fluoride substrate in atmospheric conditions at a temperature of 110°C is considered.

Figure 7-17: Bubble size after 8 ms into the simulation, for different levels of mesh refinement. The case of a single steam bubble nucleating on a calcium fluoride substrate in atmospheric conditions at a temperature of 110°C is considered.

7.2.5 Influence of thermal conductivity of the substrate on modelled bubble growth

A sensitivity study has been conducted to find the likely importance of the uncertainty of the substrate thermal conductivity on computed bubble growth. A parametric study was conducted, whereby the driving temperature difference was set 10K, and evaporative
resistance was ignored. Values of thermal conductivity between the plausible range 10-70 W/m/K have been used, as in the 1D model previously described.

Results highlighted the sensitivity of bubble growth rate (Figure 7-18) and microlayer evaporation rate (Figure 7-19, Figure 7-20, Figure 7-21) to the value of thermal conductivity. This is a consequence of the importance of conjugate heat transfer as regards microlayer depletion. The observed variation in computed evaporation rates is consistent with what emerged from the 1D analysis discussed in the preceding text.

Figure 7-18: Effect of variation of the thermal conductivity of the substrate on computed bubble size.
Figure 7.19: Effect of variation of the thermal conductivity of the substrate on cumulative mass evaporated (in milligrams of vapour) from the microlayer.

Figure 7.20: Effect of variation of the thermal conductivity of the substrate on global instantaneous microlayer evaporation rate (in milligrams of vapour per second).
Figure 7-21: Effect of variation of the thermal conductivity of the substrate on the spatially averaged heat flux from the solid to the bubble, flowing across the bubble-base area.

### 7.3 Analysis of CFD results

The shape of the bubble curved surface and the temperature distribution in the solid substrate at three times into the simulation are shown in Figure 7-22, for the case of $T_\infty - T_\Delta T = 15K$. Evaporative thermal resistance is included, set equal to $4.1 \times 10^{-6} \text{ W/m}^2/\text{K}$, following the analysis of chapter 4. The bubble grows as a truncated sphere, a typical shape observed in experiments at Jakob numbers similar to one here considered (~45) (Duan, Phillips et al. (2013), Jung and Kim (2014)). In the solid beneath the bubble base, a perturbation of the initial uniform temperature field is seen as cooling propagates into the substrate. This is due to the effect of microlayer evaporation, captured by the conjugate heat transfer incorporated.

The computed penetration depth of the temperature disturbance, judged from Figure 7-22 to be approximately 0.5 millimetres after $\Delta t = 8 \text{ ms}$, is similar to the *a priori* estimate of $\delta_{th}(\Delta t) = \sqrt{\Delta t \lambda_s/\rho_s/c_s} = 0.4 \text{ mm}$.

A magnified view of the temperature distribution in the solid beneath the bubble is shown in Figure 7-23. Here the cell-values are visible, for a discretization whereby the thickness of a solid cell is approximately equal to the penetration depth after 0.09 ms, namely 41.67 micron.
Figure 7-22: Bubble shape and temperature distribution in the substrate at three times into the simulation of a steam bubble growing on a thermally thick solid substrate.
Figure 7-23: Microlayer thickness, heat flux of evaporation and temperature distribution in the substrate at three times into the simulation of a steam bubble growing on a thermally thick solid substrate as computed by the microlayer sub-grid scale model. Note the length scale; the bubble base size is a few millimetres, much larger than the microlayer thickness.
Also shown is the radial distribution of axial heat flux (blue line) at the solid-fluid interface, and the microlayer thickness (red line), as computed by the sub-grid model coupled with the thermal response of the solid. As the film evaporates, its depletion is accompanied by the creation of a dry-patch. A peak in the heat flux distribution is observed adjacent to the dry patch, where the liquid film thickness vanishes. Within the dry patch and outside the bubble base, the heat flux is negligible compared to the value observed beneath the microlayer.

7.3.1 Effect of evaporative resistance on bubble expansion

In Figure 7-24, the effect on bubble formation of including evaporative resistance in modelling microlayer evaporation is explored. Shapes of the bubble-curved surface are shown at three times, as computed with (red line) and without (blue line) evaporative resistance. The three rows correspond to three different driving temperature differences \((T_m - T_{SAT})\), of (from top to bottom) 5, 10 and 15 K.

![Figure 7-24: Influence of evaporative thermal resistance on the bubble growth computed by the ITM.](image)
A significant difference in computed bubble volume is observed if the resistance to evaporative heat transfer is incorporated, Figure 7-25.

It will be recalled that the phenomenon is not taken into account in computing evaporation from the bubble-curved surface, as this was shown to be adequate in chapter 3. Therefore, the observed discrepancy is due to the effect of evaporative resistance on production of vapour from the microlayer, which is seen to be important, Figure 7-26.

Variations in microlayer evaporation change the bubble growth rate via two mechanisms. Firstly, this is due to the change in the contribution to bubble expansion of the vapour itself produced via microlayer evaporation. Secondly, at equal vapour production per unit area \([\text{m}^3/\text{m}^2/\text{s}]\) from the bubble curved surface, an increase in microlayer evaporation causes an increase in surface area of the bubble wall, which leads to an increase in the evaporation rate \([\text{m}^3/\text{s}]\) at the bubble wall.
Figure 7-26: Cumulative vapour production from the microlayer, for different temperature differences driving bubble growth, with and without inclusion of evaporative thermal resistance.

From Figure 7-27, microlayer evaporation appears to be the dominant contribution to bubble formation; therefore the first, direct mechanism seems to be dominant.

Figure 7-27: Comparison between total (microlayer plus curved surface) cumulative vapour production, and from the microlayer alone, during steam bubble growth at atmospheric pressure at a superheat of 15 degrees above saturation.
7.4 Microlayer evaporation rates

The effect of the additional resistance to the flow of heat here introduced on the process of microlayer evaporation, its depletion, and on the formation of a dry patch is here analysed. The case of $T_{\infty} - T_{\text{SAT}} = 15 \, K$ is considered.

In Figure 7-28 the evaporative flow of heat into the bubble from its base is shown, computed based on microlayer evaporation rate and bubble base area as

$$\text{average heat flux} = \frac{\dot{m}}{S_b} h_s = [W/m^2]$$

(7.8).

It is clear that this flow of latent heat into the bubble from its base is not much affected by the evaporative resistance, except for the early stages of growth (until approximately 1 ms). The discrepancy is no larger than 15% during most of bubble expansion. However, the bubble volume has been shown to be much affected.

This behaviour is likely to be due to a feedback mechanism, as follows. The production of vapour from the microlayer (evaporated mass or volume per unit time, or equivalently the associated flow of latent heat) can be thought of as the product of the average mass flux
(equivalent to the heat flux of Figure 7-28) times the bubble base area. The latter is the ‘active’ area available for microlayer evaporation. A decrease in the latent heat flux causes a decrease in the expansion rate of the bubble, and therefore of the bubble base. This is in effect a decrease of the area available for microlayer evaporation. As a consequence, the global evaporation – which inflates the bubble – decreases, meaning a decreased rate of expansion of the bubble base, and so on. The large effect of evaporative resistance on microlayer evaporation seen in Figure 7-29 is thus mainly due to the increase in bubble base area, Figure 7-30, in an indirect way. The difference in bubble base area is mainly determined by the initial growth (during which the discrepancy in bubble base expansion rates is large). This initial large difference in growth rate is likely a consequence of the large discrepancy of microlayer heat fluxes observed at the beginning of bubble expansion.

![Diagram](attachment:figure.png)

Figure 7-29: Time history of the instantaneous global evaporation rate from the microlayer, during steam bubble growth at atmospheric pressure at a superheat of 15 degrees above saturation.
7.5 Comparison with measurements

7.5.1 Measurements of microlayer depletion

A set of data of bubble growth and microlayer evolution (Jeong, Jung et al. (2015)), similar to that analysed in chapters 5 and 6, is used for comparison with the model described in the preceding text. The experimental arrangements are the same as the ones already described. What matters for present purposes are the measurements of time histories of bubble base radius, dry patch radius, and of the spatial variation of microlayer thickness. Data on the growth of four bubbles were collected, as summarised in Table 7-2. Useful repeatability of the measurement was achieved, as shown in Figure 7-31. Here, the bubble departure time is taken as the time when the bubble base radius (‘microlayer radius’ in the figure) vanishes. Similarly, the microlayer depletion time is taken as the time when the dry patch radius and the bubble base radius become equal. The time history of the spatial variation of film thickness is shown in Figure 7-32.
Table 7-2: Bubble growth parameters used for comparison with bubble-growth simulation in conditions for which microlayer evaporation contributes significantly to bubble-growth. Data from (Jeong, Jung et al. 2015).

<table>
<thead>
<tr>
<th>Bubble #</th>
<th>Surface Temperature [°C]</th>
<th>Microlayer depletion time [ms]</th>
<th>Bubble departure time [ms]</th>
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<tr>
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<td>14.0</td>
<td>24.3</td>
</tr>
<tr>
<td>4</td>
<td>119.3</td>
<td>11.2</td>
<td>23.1</td>
</tr>
</tbody>
</table>

Figure 7-31: Measured bubble base radius and dry patch radius as a function of time, in conditions of the data of Table 7-2.
Figure 7-32: Time history of measured microlayer thickness as a function of the distance from the centre of the bubble base, in conditions of the data of Table 7-2.

7.5.2 CFD model of bubble growth and detachment

The bubble-growth simulation has been carried out in conditions representative of bubble number three of the experimental data set, whereby the incipient nucleation temperature is equal to 119.6 °C. The need to accommodate bubble lift-off required a larger domain than that used in the simulations presented so far. Keeping the same discretization (cells of side 41.67 micron) and boundary conditions, the total number of cells needed was 11,375,616.

The heat input from the ITO heater, corresponding to an average input heat flux of 200 kW/m², was modelled as a volumetric source present in the uppermost layer of cells in the solid. An initial temperature distribution representative of pool boiling was adapted from the correlation by Nishikawa and Fujita (1977):

\[
T' = 1 - \xi \quad (0 \leq \xi \leq 0.5) \\
T' = \frac{0.257}{\left(\xi^{3/2} - 0.0883\right)^{1/2}} \quad (\xi > 0.5)
\]  

(7.9)
where non-dimensional vertical distance from the heat transfer surface is \( \xi = z/d_T \). The superheated layer thickness \( d_T \) is computed according to

\[
Nu^* \frac{d_T}{l} = B
\]

(7.10),

being \( l \) the characteristic dimension of the heat-transfer plate (12.5 mm in this case). Following Nishikawa et al., the empirical constants \( S \) and \( B \) were taken to equal to, respectively, 0.5 and 0.292.

A hydrophilic condition is imposed in the wall adhesion model, corresponding to an equilibrium contact angle of 0°.

### 7.5.3 Modelled and measured microlayer depletion

Computations have been repeated varying the evaporative resistance within a ±15% range around its inferred value. This was required in order to have an indication of the influence of uncertainties in the inferred evaporation heat transfer coefficient value on modelled microlayer depletion. The influence is moderate but non-negligible, as shown in Figure 7-33, where the dry radius and the outer microlayer radius are plotted. These can be compared with the measured dry and microlayer radii, shown in Figure 7-31. Reasonable agreement between computation and measurement is observed. In particular, there is good accord between the modelled and measured bubble departure time. Also the computed time history of the dry radius is close to the experimental values, as shown in Figure 7-34.
Figure 7-33: Simulated microlayer depletion during steam bubble growth. Time histories of the dry radius are colored in red and time histories of the bubble base radius are colored in black. See Figure 7-31 for comparison with measurement.

Figure 7-34: Comparison between modelled and measured time histories of the dry patch radius during bubble-growth simulation in conditions for which microlayer evaporation contributes significantly to bubble-growth
Similarly, the predicted time history of the spatial variation of microlayer thickness is in reasonable agreement with the experimental values, Figure 7-35.

Figure 7-35: Computed time history of microlayer profile during bubble-growth simulation in conditions for which microlayer evaporation contributes significantly to bubble-growth.

7.6 Closing Remarks

The evidence for the imperfection the evaporative process, from the micro layer observations of Jung and Kim, seems fairly strong. In this chapter we have explored the influence on the macroscopic predictions of bubble growth caused by the inclusion of less than perfect evaporation in the modelling of the micro layer.

The effect is seen to be quite significant, from a combination of the fact that the rate of evaporation per unit area of micro-layer is reduced, but also that this reduced evaporation per unit area in turn results in a smaller micro layer being generated.

Comparison of observed bubble growth rates and micro-layer characteristics from the experiments seem to be reproduced reasonably well with this particular computational treatment of the microlayer. Future investigations will have to focus on a broader range of conditions.
CHAPTER 8
TRANSIENT COOLING OF THE BOILING SURFACE AT BUBBLE RELEASE

This chapter opens with an overview of the limitations of current component scale modelling of boiling, and in particular of the RPI heat flux-partitioning approach, widely used in the industry to model wall-to-fluid energy transfer. The ‘quench’ – i.e. transient conduction to cold fluid after bubble release – component of the RPI model is then analysed with a mechanistic model, based on CFD with ITM, of bubble formation and release. Large differences between the heat transfer rates predicted by the models invariably incorporated in RPI, and those computed via this mechanistic CFD treatment are observed.

8.1 Overview of practical component-scale modelling of boiling and its limitations

Practical modelling techniques require a description of wall-boiling suitable for incorporation in the analysis of systems containing large populations of bubbles, representative of boiling on real surfaces. The need is particularly pressing for the design and characterization of water-cooled nuclear reactors. Modelling is necessarily heavily empirical. Today modelling is based on phase-averaged (Ishii (1975)) CFD approaches (Niceno, Sato et al. (2010)), requiring empirical closure relations for vapour-to-liquid and wall-to-flow mass, momentum and energy exchanges. These are typically embodied in about twenty closure laws, including bubble drag and lift forces, liquid-to-vapour local heat transfer, bubble departure diameter and frequency, vapour generation rate, bubble condensation, breakup and coalescence. Besides being based on empirical correlations, the approaches typically assume idealized geometries of the vapour-liquid interface. The most widely used closure relations accounting for wall-to-fluid energy transfer are based on a heat flux partitioning approach (Kurul and Podowski (1990)), an inevitably approximate representation of the heat transfer modes associated with the growth, release and advection into the flow of steam bubbles.

The physical reality of the situation is more complex (Chatzikyriakou, Buongiorno et al. (2011)). The geometry of the liquid-vapour interface is irregular and its nature is dynamic, Figure 8-1. The mechanisms of interaction of a bubble with the solid surface depend on the
formation of liquid layers, conjugate heat transfer with the substrate, and contact line dynamics. The growth and release processes depend on the balance of surface forces, buoyancy and drag, and differ greatly depending on fluid properties and operating conditions. Once advected into the flow, the bubble surface experiences deformation due to viscous stresses and dynamic forces, and condensation, coalescence or break-up can occur. In order to gain better understanding of the processes, there is need of physically based mechanistic models based on ITM.

Figure 8-1: Boiling flow, from Chatzikyriakou, Buongiorno et al. (2011).

8.2 Heat flux partitioning – the RPI model

The heat flux partitioning model of Kurul and Podowski (1990) was developed in order to achieve closure of the thermal problem, via formulation of a semi-mechanistic law of wall-to-fluid energy exchange applicable to wall-boiling conditions. Closure is represented by a relationship between wall heat flux and the temperature difference between wall and ‘bulk’ fluid, in other words a heat transfer coefficient. It is possible to express the desired relationship via a suitable combination of nucleation site density, bubble departure diameter, and bubble release frequency. For each nucleation site, the total energy transferred from wall to fluid during one bubble cycle is decomposed into three contributions Figure 8-2:

- Evaporation, i.e. the latent heat required to form a bubble
- Energy exchanged via ‘ordinary’ single phase convection from the surface between nucleation sites
- ‘Quench’, the term used to denote energy exchange after bubble lift-off via transient conduction to the liquid.

![Quench diagram](image)

Figure 8-2: Heat flux partitioning model of nucleate boiling heat transfer.

Simple algebraic expressions can be used to quantify these energy transfers. The three components are scaled taking into account the fraction of wall area where they are assumed to be active, and converted into a heat flux via the bubble release frequency. The quench and convection components depend on the unknown wall temperature. In order to close the problem, the input wall heat flux is equated to the sum of the partitioned fluxes, which achieves the required closure of the problem:

\[
q''_w = q''_ev + q''_co + q''_q
\]  

(8.1)

Incorporation of the closure relation in the wall-boiling treatment (i.e. determining the ‘bulk’ fluid temperature, updating the wall temperature) depends on the specific CFD method and on conditions it is applied to.

The RPI heat flux-partitioning model is usually applied to forced convection boiling flows, of industrial interest. Its formulation is however equally suited for pool boiling. The fundamental understanding of forced convection boiling flows is however still incomplete. On the other hand, pool boiling in laboratory conditions has being studied extensively and is better understood. In this chapter we will thus focus on the comparison between ITM and RPI predictions applied to a pool boiling model problem.

8.2.1 Evaporative heat flux

This heat flux component accounts for the latent heat exchange due to steam bubble formation. The energy required to grow a bubble (the ‘joules per bubble’) is the product of the
bubble mass times the latent heat of evaporation. This is most conveniently expressed as a function of the bubble release diameter, for which several correlations are available:

\[ q_{ev} = \frac{\pi}{6} D^3 \rho_v h_f g \]  

(8.2).

The corresponding heat flux is obtained introducing nucleation site density and bubble release frequency:

\[ \dot{q}_{ev}'' = \frac{\pi}{6} D^3 \rho_v h_f N_s N_t \nu \]  

(8.3).

Both the site density and the release frequency are in truth only able to be predicted with large uncertainties.

8.2.2 Convective heat flux

This component represents convective heat transfer to the liquid across the wall area not occupied by the bubbles, in between nucleation sites. The hypothesis is that this process can be quantified with a convective heat transfer coefficient for single-phase convection, which does not include the influence of bubble-induced agitation of the liquid on the convective process. To this end, several correlations developed for natural and forced convection are available, such as the one by McAdams (1945) for turbulent natural convection on an upward-facing horizontal surface. The convective heat flux is related to the difference in temperature between wall and bulk as:

\[ \dot{q}_{conv}'' = \left(1 - A_b \right) h_{conv} \left(T_w - T_{bulk} \right) \]  

(8.4),

where the area fraction \( A_b \) describes the area of influence of the bubbles, and its complement is the area where single-phase convection is assumed. \( A_b \) is usually expressed as a function of nucleation site density and bubble lift-off diameter.

8.2.3 Quench heat flux

This component accounts for transient conduction heat transfer, occurring after the superheated liquid layer has been disrupted by bubble release. The hypothesis is that the departing bubble acts as a micro-pump, pushing towards the wall liquid at the remote
temperature, or at least at a temperature lower than that otherwise in such close proximity to the wall, Figure 8-3.

We follow here the development of Han and Griffith (1965). Under the hypothesis of constant wall temperature, it is assumed that cooler liquid drawn in by disruption of the thermal boundary layer is instantaneously put in contact with the wall after bubble lift-off. Heat diffuses into the liquid, which is treated as a semi-infinite thermal conductor, from the surface, which is modelled as being of constant temperature.

A simple expression for the wall heat flux can be derived from solution of the 1D Fourier equation, solved in the liquid with a Dirichlet boundary condition representing the constant temperature wall (Carlslaw and Jaeger (1959)):

\[
q''(t) = \frac{\lambda(T_w - T_q)}{\sqrt{\pi \alpha_t t}}
\]  

(8.5).

In order to derive the RPI-partitioned quench heat flux, firstly the instantaneous heat flux is integrated over the bubble release period to obtain an energy fluence [J/m²] per bubble:

\[
q'' = \frac{2\lambda(T_w - T_q)}{\sqrt{\pi \alpha_t}} \sqrt{\tau}
\]  

(8.6).

The model requires postulating an area of influence of the quench flux, which is usually chosen as a circle of diameter equal to twice the bubble characteristic dimension, \(D_D\), at departure, as suggested by Han and Griffith (1965).
The product of the fluence times the area of influence physically represents the ‘energy per bubble’ transferred to the fluid by the quench mechanism.

The RPI-partitioned quench heat flux itself is simply the product of quench energy per bubble, bubble release frequency and nucleation site density:

\[
q''_q = \frac{2\pi \lambda \left(T_v - T_q\right)}{\sqrt{\pi \alpha_l}} \sqrt{\nu D^* N^*_{sle}}
\]  

(8.7)

There are several limitations to this approach:

- The thermal response of the solid, and hence the temperature distribution around the nucleation site, are not accounted for.

- In addition, there is no rigorous criterion to assign the correct portion of wall area to the transient conduction heat transfer mechanism.

- The liquid modelled as being brought into sudden contact with the wall is treated as being stationary, semi-infinite, and of initial uniform temperature.

- Finally, the ‘quench’ temperature of this liquid, needed in order to model the transient conduction energy transfer, is an uncertain parameter.

It is worth noting that this ‘quenching’ is generally believed to be of considerable significance. Han and Griffith (1965) (and, later, Mikic and Rohsenow (1969)) concluded that quench transient conduction is the main contributor to the overall pool boiling heat transfer. Kubie (1975) investigated the interaction of a heated platinum wire with an adiabatic column of air bubbles, and deduced that transient conduction following the interaction of a bubble with the wire was by far the dominant heat transfer mechanism. Similar conclusions were reached by Gerardi, Buongiorno et al. (2010), via post-processing of boiling curves extracted from pool boiling experiments of water at atmospheric pressure. Boiling-curves obtained at different heat fluxes were decomposed into the RPI heat flux components (Gerardi (2009)), using the measured nucleation site densities, frequencies, and lift-off sizes. The quench component was found to be the largest, Figure 8-4.
8.3 Mechanistic approach to modelling quench heat flux

The development of a steam bubble at a heated surface, sketched in Figure 8-5, is simulated with the ITM methodology described in the previous chapters. As an initial condition, a seed of vapour is placed at the centre of the heated surface, its location termed a nucleation site. The pocket of vapour grows due to the addition of heat from the surrounding fluid and from the substrate, and detaches at a size much greater than its initial radius (which is magnified in the illustration for visibility), the influence of its initial magnitude on the eventual computed lift-off size being therefore negligible. During bubble development, energy is removed from the solid and from the superheated near-wall liquid. However, due to its large thermal capacity, at bubble lift-off the temperature in the solid is still higher than the remote liquid temperature. The phenomenon here under investigation is the detachment of the steam bubble, and the sudden contact between the hot solid surface and the liquid, the latter presumably at a temperature not very different from that of the remote liquid.
8.4 The model problem

An average input heat flux of 50 kW/m², typical of the ‘isolated-bubbles’ boiling regime at atmospheric pressure, is considered. At such a low (so far from the CHF condition) heat flux, the occurrence of boiling on real surfaces is characterized by the nucleation of bubbles at preferential locations, typically separated by a distance comparable to the bubble lift-off size. The distribution of potential nucleation sites presumably depends on the features of the boiling surface (Carey (1992)), or on the presence of nanoscopically small voids (‘nanobubbles’, Lohse and Zhang (2015), Nam and Ju (2008)). Bubble formation occurs at a site depending on the thermal response of the solid, i.e. depending on the local nucleation mechanisms; for example, given the features of a specified surface defect, a bubble is observed to grow there once the local temperature has exceeded a certain value (Witharana, Phillips et al. (2012)). A single unconstrained bubble, free to grow at a horizontal surface in an extended pool of liquid is considered, shown in Figure 8-6. The initial temperature at the heat transfer surface is set equal to 120°C, a typical bubble nucleation temperature observed in laboratory conditions (Jung and Kim (2014)).
8.4.1 Evaluation of RPI-partitioned quench cooling rate for the model problem

Figure 8-7 shows the energy fluence obtained applying the transient conduction sub-model outlined in section 8.2.3 to the model problem here considered; that is with the wall at 120 °C, and the remote liquid at 100 °C.

Figure 8-7: Local heat flow due to transient conduction to fluid at the remote temperature, following bubble release, computed by applying the model of Han and Griffith.
In order to compute the corresponding energy transfer, it is assumed that a circular area of wall, of diameter equal to the twice the characteristic bubble lift-off size, is brought into contact with liquid at the remote temperature, as prescribed by the treatment. This factor of two is typical of that applied in RPI modelling.

For water at atmospheric pressure, a plausible value of the lift-off diameter in pool boiling conditions is 4-5 mm (see for example Duan, Phillips et al. (2013) and Jung and Kim (2014)). The evaporation energy transfer corresponding to the formation of a 4 mm bubble is approximately 60 mJ.

![Energy transfer graph](image)

Figure 8-8: Energy transfer across the area where the transient conduction heat transfer mechanism takes place, computed by applying the model of Han and Griffith.

From Figure 8-8, it is clear that within a few milliseconds after lift-off, the computed quench energy transfer has already exceeded the ~ 60 mJ evaporation energy transfer.

8.4.2 Mechanistic model of isolated bubbles pool boiling

We now turn to the CFD setup used to simulate bubble formation. It was chosen to simulate only one quadrant of the physical domain for the production runs, using symmetry boundary conditions. The computational domain, where the three-dimensional unsteady heat and fluid
flow equations are solved, consists of a square based parallelepiped, of dimensions shown in Figure 8-9. The size of the domain was set as the smallest that yielded size-independent results. The solid domain depth was chosen by evaluation of the typical thermal penetration depth based on the characteristic bubble release period in the conditions of interest. An appropriate thickness – equal to a few penetration depths – was chosen in order to nullify the influence of the effect of the bottom boundary of the domain. The material properties of stainless steel have been used making the thermal effusivity of the solid about six times that of the working fluid. This value is typical of boiling conditions. The heat input is modelled as fixed heat flux, applied at the underside of the steel.

A uniform discretization is adopted in the fluid region where the bubble develops; away from it, where the details of the flow are less important, the mesh is stretched to reduce computational cost. In the solid beneath the bubble, cells with higher aspect ratio are used to capture the vertical temperature gradients.

**Figure 8-9:** ITM model of single bubble growth during pool boiling: dimensions of computational domain.

### 8.4.3 Boundary and initial conditions

Flow of heat and mass is not allowed across the four side boundaries, as indicated in Figure 8-9. Flow of mass out of the domain is allowed across the top boundary, whose temperature is specified as a ‘faraway’ liquid temperature (100 °C in this case). A constant heat flux of 50 kW/m² is applied at the bottom boundary. The initial temperature in the solid was set to vary linearly between the value $T_w = 120^\circ$C at the solid-fluid interface, and the value $T_0 = T_w + \ldots$
\( q'' \) being \( q'' \) the imposed heat flux and \( l \) the solid slab thickness. The fluid is initially stagnant. The initial seed of vapour is placed at the solid-fluid interface at the intersection of the \( x=0 \) and \( y=0 \) planes. The initial temperature distribution in the fluid is computed according to the correlation by Nishikawa and Fujita (1977), as described in Chapter 5.

### 8.4.4 Mesh sensitivity study

#### 8.4.4.1 Hydrodynamic problem

Details of the flow at bubble lift-off are important since they determine how readily the fluid at the remote temperature can reach the heated surface. To elucidate the sensitivity to discretization of the hydrodynamic aspect of the problem under investigation, the study was run without solving the energy equation, and with no evaporation model (neither mechanistic, as that used for evaporation at the bubble surface, nor modelled, as the one used to compute microlayer depletion). The volume of the bubble was increased imposing a spatially uniform, but time-dependent, volumetric source of vapour in the cells containing the interface. The source rate has been tuned in order to obtain a plausible bubble detachment size, 4.5 mm in this case, and was deactivated once the bubble lifts off. Three levels of uniform discretization were chosen, corresponding to cubic cells of side equal to, respectively, 250, 125 and 62.5 micron. Details of the flow field are shown in Figure 8-10, where velocity vectors of equal length, but coloured according to their magnitude, are shown, from top to bottom, at 19, 21 and 23 ms into the simulation.
Figure 8-: Mesh sensitivity of the hydrodynamics of bubble detachment.
The hydrodynamics here under investigation seem weakly dependent on the adopted discretization, as indicated by the small discrepancy in bubble shape, direction and magnitude of the velocity vectors observed if the two finer meshes are compared.

8.4.4.2 Hydrodynamics and heat transfer

The CFD calculation computes the conductive heat flux at the metal-liquid interface at every cell and at every time step, allowing the ready extraction of quantities such as spatial and temporal integrals. The start of the rewet-quench process is here taken as the time of full depletion of the microlayer. The quench energy transfer is computed as the energy fluence times the surface area of the quench-affected portion of wall.

A comparison between the time histories of energy transfer, evaluated at the quench area of influence and computed with several levels of discretization, is shown in Figure 8-11. The levels of discretization considered are summarised in Table 8-1, where $\Delta x_f$ is the mesh size in the fluid, and $\Delta z_s$ is the thickness of a solid cell. The time histories of energy transfer were found to depend on the discretization to a greater degree than did the flow field, as is apparent also from Figure 8-12, where the cumulative energy transfer at 10 ms from the initiation of the rewet process is shown.

<table>
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<td>7.81</td>
<td>208×208×852</td>
<td>36,860,928</td>
</tr>
</tbody>
</table>

Table 8-1: Parameters of mesh sensitivity analysis of the ITM model of single bubble growth during pool boiling.
Figure 8-11: Mesh sensitivity analysis of the ITM model of single bubble growth during pool boiling: computed time histories of quenching energy transfer as a function of mesh refinement.

Figure 8-12: The energy extracted after 10 ms of quenching of the solid substrate after bubble release as a function of the level of discretization.

Sensitivity of the computed quench energy transfer to the number of mesh points used is seen to decrease with increasingly fine discretization (levels 4, 8 and 16).
8.5 CFD results and analysis

8.5.1 Qualitative analysis of bubble growth and lift-off

Bubble shape and temperature distribution in the solid and in the fluid at a vertical plane containing the nucleation site are shown in Figure 8-13. Results are shown at several times before and after the moment of bubble lift-off. A horizontal black line denotes the solid-fluid interface, while the bubble wall is represented by a white line.

The bubble initially grows as a hemispherical cap, with the base diameter and the bubble height growing more or less at the same rate, inflated by evaporation from the superheated liquid layer and from the microlayer. Evaporation of this thin liquid film causes local cooling of the wall at the bubble base, where typical heat fluxes at the solid-fluid interface are of order 1 MW/m². The heat flux is negligible where the solid is in contact with vapour, at the dry patch beneath the bubble.

After approximately 15 ms the microlayer has evaporated completely, and the bubble base is now entirely dry. The contact line modelled by the interface tracking methodology now has a physical significance, being the actual triple line of separation between the solid-liquid and solid-vapour interfaces. A hydrophilic condition, namely a contact angle of zero degrees, is imposed in the wall adhesion model governing the motion of the contact line. This choice has been originally proposed, for nucleate boiling simulations, by Sato and Nićeno (2015); good agreement between measured and computed bubble lift-off was observed in such cases. The combination of buoyancy and wall adhesion forces eventually causes bubble detachment. This is accompanied by an advancing liquid front, as the circumference of the base of the bubble reduces, which covers with liquid the dry patch that was previously exposed to vapour. Typical heat fluxes observed during cooling of the dry patch by the advancing liquid front are up to 350 kW/m², and the process lasts for a few milliseconds. It is interesting to observe that, taken literally, this is the ‘quenching’ process, and is associated with relatively low heat fluxes.

A close-up of the flow field during the detachment process is shown in Figure 8-14. Liquid rushes in, filling the space previously occupied by the vapour, predominantly from the near-wall superheated layer, which is at a higher temperature than the remote liquid.
Figure 8-13: Bubble shape and temperature distribution in the solid and in the fluid at a vertical plane. From top left to bottom right, times are 0, 6, 12, 18, 22 and 36 ms after nucleation.
Figure 8-14: Velocity field during lift-off, preceded by the reduction in bubble base radius and ‘quenching proper’. From top to bottom, times are 16, 18, 20 and 22 ms.
During bubble expansion, the locally varying time-dependent heat transfer at the bubble base is rather complicated. By construction, at the outward-moving edge of the bubble base, an imposed radially-increasing thickness of water film is left behind. It will be recalled that the layer is not resolved by the computational grid; it has to be regarded as a ‘virtual’ film, whose depletion is tracked by the dedicated sub-model. Meanwhile, a dry patch at the centre of the bubble base is created, by evaporation computed within this sub-model, and increases in radius due to the progressive depletion of the microlayer. Bubble shape, temperature distribution in the substrate and modelled microlayer slope are shown in Figure 8-15 at two times, namely 4 and 10 ms, into bubble expansion.

The typical radial variation of heat flux at the solid-fluid interface during this phase of bubble growth is shown in the top panel of Figure 8-17, together with the bubble shape and the temperature distribution in the solid.
Figure 8-15: Bubble shape, and temperature distribution in the solid, as predicted by the CFD method. These are shown together with the microlayer thickness, as computed by the dedicated algebraic sub-model. Note the length scale; bubble size is a few millimetres, much larger than the microlayer thickness.
Later on, bubble release occurs. A close-up view of the flow and temperature field during the detachment process is shown in Figure 8-16. The liquid rushing in, filling the space previously occupied by the bubble, is from the near-wall superheated layer, which is at a higher temperature than the remote liquid.

Figure 8-16: Velocity and temperature field during lift-off, preceded by the reduction in bubble base radius and ‘quenching properly’. The vapour-liquid interface, seen after 16 and 20 ms into the simulation, is represented as a red line. Only the fluid domain is shown in the diagram. The temperature field, in degrees Celsius, is shown in grey-scale, velocity vectors are colored according to their magnitude (in m/s). Small flow velocities are observed in the image taken at 36 ms, showing superheated liquid (light grey) in motion towards the nucleation site.
Neither the flow field nor the time-dependent temperature distribution shown in Figure 8-16 is suggestive of liquid at the remote temperature rushing in, from a region where it was at some ‘bulk’ temperature, towards the hot wall, and causing vigorous quenching.

On the other hand, vigorous cooling of the substrate, not unlike that occurring during microlayer evaporation, is observed during detachment, as the dry patch is covered by liquid, as shown in the middle panel of Figure 8-17. This might be due to either a transient conduction process into a ‘thick’ body of liquid, or to quasi-steady conduction through a thin layer of liquid, bounded at the top by the liquid-vapour interface (which is at the saturation temperature). The typical penetration depth in the liquid after a time comparable to that taken by the rewet front to cover the dry surface (a few milliseconds) is of several tens of microns. The liquid depth between the saturated liquid-vapour interface and the wall reaches up to a few hundreds of microns, but it decreases to zero over a fraction of a millimetre (see the steep slope of the liquid-vapour interface close to the wall). However, the solid is initially in contact with the smaller thickness of liquid. Given the small flow velocities observed, and the thickness of liquid between wall and vapour-liquid interface, conduction remains the only possible heat transfer mechanism, but it is not possible to demonstrate whether the thermal capacity of the liquid plays any role. We will return to this point. Given plausible values of the thickness of liquid in contact with wall (of up to ~100 microns), and the wall temperature at the dry patch (approximately 117 °C, from Figure 8-15), the heat flux due to quasi-steady conduction is of order hundreds of kilowatts per square meter, not unlike that extracted from the mechanistic simulation. However, previous analyses have modelled the heat flow during bubble detachment as transient conduction, see Demiray and Kim (2004) and Moghaddam and Kiger (2009).

Whatever the mechanism, enhanced cooling of the solid substrate during rewetting of the dry area previously in contact with vapour, and now quenched by the liquid, is clear. Bubble shape and radial heat flux profiles are shown at three times during the rewetting process in Figure 8-18. A local increase in heat flux is observed as the rewetting front approaches the centre of the dry patch. Typical radial variation of heat flux at the solid-fluid interface immediately after bubble departure is indicated by the bottom panel of Figure 8-17. The heat flow has now decreased, following full covering of the dry patch by the liquid.
Figure 8-17: Example of temporal variation of typical radial heat flux profiles at the solid-fluid interface during bubble growth (top panel), bubble detachment (middle panel), and after bubble lift-off (bottom panel).
8.5.2 Extraction of quench heat flux

Direct inspection of the time dependent flow and temperature field revealed a circularly symmetric temperature distribution at the heat transfer surface during and after bubble lift-off.

The local instantaneous flow of heat from the substrate to the liquid is monitored along a line probe, at a sequence of times, Figure 8-19.
Inspection of instantaneous radial heat flux profiles showed a perturbation of the ordinary convective background – that imposed by the initial temperature distribution – localised in an area significantly smaller than that of a circle of diameter equal to twice the bubble lift-off size (the region normally considered subject to ‘quench’ in the RPI approach). This is evident in Figure 8-20, where the green vertical line represents the maximum bubble base computed by the interface tracking method, the purple line denotes the lift-off radius – also computed mechanistically, and the pale blue line represents the radius of the quench area of influence of the transient conduction model of Han and Griffith for this lift-off radius.

Figure 8-20: Area of influence of the quench energy transfer.
The characteristic diameter of the actual quench-affected circular area is more similar to the maximum bubble base diameter than to the lift-off diameter. The temporal variation of both of these are shown in Figure 8-21.

Figure 8-21: Time histories of computed bubble base and equivalent diameter for the pool boiling model problem considered.
8.5.3 Influence of material properties of the substrate

Computations have been repeated for different substrates, including high-conductivity materials such as copper and aluminium. Thermal conductivity $\lambda$, specific heat capacity $c$ and density $\rho$ of the solids here considered are listed in Table 8-2.

<table>
<thead>
<tr>
<th></th>
<th>Steel</th>
<th>Copper</th>
<th>Aluminium</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda \left[ \frac{W}{mK} \right]$</td>
<td>14.0</td>
<td>401.0</td>
<td>227.0</td>
</tr>
<tr>
<td>$c \left[ \frac{J}{kgK} \right]$</td>
<td>490.0</td>
<td>385.0</td>
<td>940.0</td>
</tr>
<tr>
<td>$\rho \left[ \frac{kg}{m^3} \right]$</td>
<td>7700.0</td>
<td>8960.0</td>
<td>2700.0</td>
</tr>
</tbody>
</table>

Table 8-2: Material properties of substrates investigated in the assessment of the transient conduction cooling of the boiling substrate at bubble release.

The largest ‘quench’ energy transfer, computed via the line probe approach, is observed for the high-conductivity materials such as aluminium and copper, Figure 8-22, although it is noteworthy that there is broadly a factor of two between stainless steel and copper, although their conductivities differ much more.
Larger bubble dimensions were observed for the higher thermal conductivities, Figure 8-23.

This causes by itself an increase in the quench energy transfer, by increasing the affected area. However, some increase in the energy exchanged per unit area for increasingly large thermal conductivities of the solid was observed, Figure 8-24.
For the case of copper, the maximum temperature drop at the solid-fluid interface was less than 5% of the initial superheat (20°C). Larger heat flow rates have been observed during rewet of the effectively isothermal copper surface, as seen in Figure 8-25 (see Figure 8-18 for comparison for the case of a steel substrate). Notably, the peak heat flux achieved during the rewet phase of the high-conductivity substrate is of the same order of magnitude of that observed under the microlayer during bubble growth.
Figure 8-25: Spatial and temporal variation of the heat flux at the solid-liquid interface during rewet of the wall dry area during boiling on a high thermal conductivity surface.

Imposition of an isothermal surface is a convenient means to compare the rewet energy transfer with the estimates obtained applying extant models, such as the transient conduction model of Demiray and Kim (2004), and a quasi-steady conduction model developed ad hoc, to be discussed later on in the chapter.

8.6 Comparison between CFD-generated and RPI-partitioned quench heat flux

The energy transfer from wall to liquid extracted from the CFD simulation, and that resulting from application of the RPI sub-model are compared, Figure 8-26. Results obtained for the low-conductivity case of a stainless steel substrate are shown.
A discrepancy is observed. The RPI-partitioned energy fluence shows a parabolic dependence on time which is typical of the transient conduction process, and which is not exhibited by the time history of heat flow from the mechanistic simulation, which increases rapidly in a few milliseconds after microlayer depletion (the rewet process), and then increases linearly at a low rate. This is consistent with the observation that the temporal variation of the local temperature distribution does not show fluid at the remote temperature moving towards the wall as a consequence of bubble release, as discussed in section 8.5.1. On the contrary, the fluid rushing in towards the wall is significantly hotter than saturation, being drawn in from the superheated liquid layer, and this provides a less effective heat sink. Another reason for the observed discrepancy is conjugate heat transfer with a finite thermal conductivity boiling substrate (ignored in the Han–Griffith model), which has also been cooled by microlayer evaporation prior to bubble lift-off.

The axial temperature variation in the solid and in the liquid at a radial distance of 300 microns from the nucleation site (that is, well within the region that becomes dry) is shown in Figure 8-27, at multiple times during the quenching. The RPI-modelled temperature variation is taken from the 1D solution for the unsteady temperature distribution in the solid, from
Carlslaw and Jaeger (1959). The main difference between the RPI- and mechanistically-modelled axial temperature profiles is the presence of fluid, at a temperature larger than the remote value, close to the heat transfer surface. By construction, in the RPI model the surface is exposed to a body of fluid at the remote temperature.

Figure 8-27: axial temperature variation in the solid and in the liquid at a fixed radial distance from the nucleation site during bubble lift-off and subsequent ‘quenching’ of the substrate. Negative z-values indicate the solid, positive z locations are in the liquid.

The radial variation of heat flux at the solid surface is shown in Figure 8-28 at various times during the quenching. The RPI treatment asserts that cooling occurs over an area much larger than the mechanistically –computed quenching area.
Figure 8-28: radial profiles of heat flux at the solid surface from ITM and RPI modelling during ‘quenching’ of the substrate.

As a consequence, there is a large discrepancy between the overall energy transfer obtained with the two approaches, Figure 8-29, where the mechanistically-computed flow of heat is integrated over the appropriate area of influence. The quench energy transfer predicted by the Han-Griffith sub-model is orders of magnitude larger than that predicted with the present methodology. Probably the biggest contributor to this is the overestimation of the quench area of influence in the Han-Griffith treatment, where the quench area of influence is approximately sixteen times larger than that computed mechanistically.
Figure 8-29: Comparison between energy transfer from mechanistic simulation and RPI partitioned energy transfer, for the pool boiling model problem considered, for the case of a poorly conducting substrate.
A smaller discrepancy is observed for the case of the high-thermal conductivity substrate. This is to be expected, and in effect the Han-Griffith model treats the substrate as being of infinite conductivity. This is seen in Figure 8-30 and Figure 8-31.

Figure 8-30: Comparison between energy fluence from CFD analysis and RPI partitioned energy fluence, for the pool boiling model problem considered, for the case of a high-conductivity substrate.

The present analysis seems to indicate that the order of magnitude of the combined rewet/quench energy transfer is a few milli-Joules, while previous approaches predicted hundreds of milli-Joules. If the quench/rewet energy transfer is compared to the evaporation energy transfer required to form a bubble of the size observed in this investigation (4 mm in diameter, corresponding to approximately 60 mJ), our analysis indirectly suggests that the evaporation component of nucleate boiling heat transfer is a large multiple of the ‘quench’.
Figure 8.31: Comparison between energy transfer from mechanistic simulation and RPI partitioned energy transfer, for the pool boiling model problem considered, for the case of a high-conductivity substrate.
8.7 Rewet analysis

In this final section we go on to make a preliminary suggestion for a simple semi-analytical model, following in some sense the spirit of the Han and Griffith approach, but informed by the greater physical understanding that has been provided by these detailed simulations. The model is approximate, and simple to apply, and has been developed with a view to proposing it as a complement or alternative to the classical Han-Griffith approach.

The RPI quench model is predicated on the assumption that fluid at the remote temperature touches the hot metal instantaneously at the moment of bubble lift-off. A more realistic description would however acknowledge that the bubble departure process occurs during a finite time. As shown in Figure 8-18 and Figure 8-25, an advancing liquid front rewets the dry patch during this time of bubble lift-off.

8.7.1 Transient conduction model

It is required to compute the energy transfer from wall to fluid as the dry patch is covered by a liquid front, as the front advances at a finite speed, Figure 8-32.

Following the development of Demiray and Kim (2004), it is assumed that the wall dry area is progressively covered by a liquid front advancing at a constant velocity $v$. The wall temperature is assumed constant, and the thickness of liquid covering the dry patch is assumed much larger than the penetration depth based on the typical time of exposure to the liquid at locations on the surface inside the initial dry patch.
Figure 8-32: transient conduction model of the heat transfer during rewet of the wall dry area at bubble lift-off.

The liquid is initially at a uniform temperature $T_l$. Let $r_0$ be the initial dry patch radius at time $t'$. At location $r' < r_0$ and time $t$, the wall has been wetted for a time $t - t'$. The heat flux at time $t$ is

$$q(r,t) = \lambda \left( T_w - T_l \right) \frac{\pi \alpha}{\sqrt{\pi \alpha (t - t')}}$$

(8.8)
The instantaneous flow of heat [W] at time $t$ is obtained integrating in space from $r_0$ to the location $r$ where the front has arrived at time $t$, which depends on the rewet velocity $v$:

$$\dot{q}_w(t) = \frac{\lambda (T_w(T) - T_i)\int_{r_0}^{r} \frac{2\pi r'}{\sqrt{\pi \alpha_i}} \sqrt{f(r') - f(r)} dr'}{\sqrt{\pi \alpha_i}}$$

(8.9),

where $t=f(r)$ expresses the dependency on location of the time of exposure of the wall to the liquid. For the special case of constant $v$, $r = r_0 - vt$, and the power transfer $\dot{q}$ is:

$$\dot{q}_w(t) = \frac{4\pi \lambda (T_w(T) - T_i)r_0}{\sqrt{\pi \alpha_i}} \sqrt{v \left[ \frac{1}{3} (vt)^{3/2} + (r_0 - vt)(vt)^{1/2} \right]}$$

(8.10).

The cumulative energy transfer at time $t$ is obtained via time-integration of this expression:

$$q_w(t) = \frac{4\pi \lambda (T_w(T) - T_i)r_0}{\sqrt{\pi \alpha_i}} \sqrt{v \left[ \frac{2}{3} r_0 t^{3/2} - \frac{4}{15} vt^{5/2} \right]}$$

(8.11).

This expression is evaluated (Figure 8-34) using values of the rewet velocity and dry patch radius extracted from the simulation. The latter was found equal to 0.9 mm, the former, computed as the time-derivative of the instantaneous bubble base radius, exhibited a dependency on time, Figure 8-33.

![Figure 8-33: time history of advancing liquid front velocity computed with the mechanistic ITM model of steam bubble release.](image)
For simplicity, a constant value of 0.25 m/s, representative of a large fraction of the rewet transient, is assumed here.

The initial liquid temperature is varied as a free parameter, within bounding values of 100 and 115 °C.

![Figure 8-34: rewet energy transfer from transient conduction model.](image)

The energy transfer depends strongly on the initial temperature of the liquid the wall is exposed to.

**8.7.2 Quasi-steady conduction model**

The hypothesis is that the thickness of liquid covering the dry patch is variable, as indicated by results of present modelling shown in Figure 8-35, and is dictated by the slope of the vapour-liquid interface close to the wall.
Figure 8-35: quasi-steady conduction model of the heat transfer during rewet of the wall dry area at bubble lift-off.

The flow of heat is driven by the temperature difference between the upper and lower surfaces of the liquid film, respectively the liquid-vapour and solid-liquid interfaces. The former is at the saturation temperature $T_{\text{SAT}}$, the latter at a constant temperature $T_w$ of approximately 119°C, extracted from the CFD analysis. The local heat flux is:

$$\dot{q}_w'' = \frac{T_u - T_{\text{SAT}}}{l_b} \lambda$$

where $l_b$ is the local value of the thickness of liquid covering the dry patch.
The liquid film thickness \( l_b \) depends on the slope of the liquid-vapour interface at the wall, and on the rewet velocity. The particular case of constant thickness and constant rewet velocity is considered first. After carrying out the spatial and temporal integration of the local instantaneous heat flux as explained in the previous section, the energy transfer is obtained:

\[
q_{\text{sw}}(t) = \frac{2\pi \lambda}{l_b} \left( T_w - T_{\text{SAT}} \right) v \left[ \frac{r_b t^2}{2} - \frac{v t^3}{6} \right]
\]

(8.13).

It was found that, in the particular conditions here considered, the slope \( s \) of the rewetting film is constant and equal to approximately 0.66. This value might depend on conditions under investigation, but in general the assumption of a liquid thickness increasing linearly with time and with typical values of tenths of millimetres seems consistent with inspection of the bubble surface close to the wall. For constant \( v \) and \( s \), it is easy to show that at each radial location

\[
l_b = s v \left( t - t' \right)
\]

(8.14).

The energy transfer at time \( t \) is then:

\[
q_{\text{sw}}(t) = \frac{\pi \lambda}{s} \left( T_w - T_{\text{SAT}} \right) \left[ \frac{r_b t^2}{2} - \frac{v t^3}{2} \right]
\]

(8.15).

Time histories of the energy transfer predicted by the quasi-steady conduction model are shown in Figure 8-36, where predictions obtained with the constant thickness model (varying the film thickness as a free parameter) and with the variable thickness model are compared.
8.7.3 Comparison between CFD-generated and analytical rewet energy transfer

The rewet models described in the text above, and the mechanistic methodology, predict values of rewet energy transfer of the same order of magnitude.

A useful comparison between the two approaches can be made if the energy transfer obtained with the transient conduction model that assumes the liquid at saturation, and that predicted by the quasi-steady conduction model with variable film thickness are taken as bounding values. Then it is observed that the energy transfer from mechanistic simulation lies within these bounds, Figure 8-37. Due to the large slope of the liquid-vapour interface and to the large rewet speed, at locations reached by the liquid front the metal is most of the time exposed to a thickness of liquid of several penetration depths, if the penetration depth is computed based on the time of exposure of the solid surface to the liquid. Therefore, transient conduction seems a plausible heat transfer mechanism. However, it reasonable to argue that the initial temperature of the liquid to which heat is conducted is higher than saturation, being this liquid from the superheated layer. A similar observation was made by Yaddanapudi and Kim (2000), based on experiments with refrigerants.
8.8 Closing remarks

The detailed CFD simulations suggest strongly that the amount of heat transferred during the interaction of single-phase liquid with the wall as the bubble detaches and departs is very much less than that which the original Han and Griffith model would suggest.

The mechanistic simulations of steam bubbles presented in this work showed that quench flows of heat affect a portion of wall area much smaller than that assumed by the usual treatments employed for the quench component. It was demonstrated that these treatments give a significant overestimate of the heat so transferred. This is mainly due to such an overestimate of the area of influence of the quench heat flow in the RPI model. In this model, the portion of wall area affected by the bubble is assumed to be cooled by the remote liquid, at a temperature significantly lower than in close proximity to the wall. On the contrary, the mechanistic simulations showed that, following bubble release, the surface is brought into contact with liquid drawn in from the vicinity of the wall (superheated liquid layer). It is expected that this effect be most pronounced for the case of small bubbles (typical, for example, of high-pressure boiling conditions), which are almost entirely enclosed within the superheated liquid layer during their growth.
Simulations of steam bubble release from high-conductivity substrates showed that an increase in thermal conductivity of the substrate was accompanied by an increase in the energy removed from the substrate via ‘quenching’. However, the effect is small compared to the discrepancy between predictions of the Han – Griffith model and CFD modelling.

Analysis of the combination of fluid flow and temperature distributions and heat transfer predicted by the CFD have allowed us to make a preliminary proposal of a simple semi-analytical model, which might possibly serve as a replacement for or complement to the use of Han and Griffith in heat flux partitioning approaches.

(It is worth commenting that when looked into in detail, indeed the individual components within heat flux partitioning approaches actually predict heat transfers significantly different from what it is firmly believed actually take place, but that typically the overall heat transfer behaviour is quite well predicted. That relates to the combination of extensive experience-based tuning of such approaches, and the fact that by their nature, in heat flux dominated circumstances, the approach is in aggregate actually very robustly conditioned. We are conscious that indeed changing anyone part of it, on its own, can upset such hard-won harmony!)

In this respect, it is hoped that these microscopic CFD simulations are serving one of their purposes; to provide greater physical insight, and to allow the necessarily very much more simple semi-analytical, semi-empirical treatments required to be used in component scale modelling to be improved.
CHAPTER 9
CONCLUSIONS

The thesis closes with a summary of the findings of this project, and their implications as regards the fundamental understanding of boiling, and the practical modelling of boiling phenomena for industrial applications. The work carried out leads to recommendations for future investigations.

9.1 Main findings of this project

9.1.1 Steam bubble formation

A novel analytical model for predicting bubble-growth due to evaporation at the bubble wall was presented. The principal advancements in the treatment are inclusion of the effects of the non-uniform temperature distribution in the liquid in which the bubble grows, and of the departure from sphericity of the bubble shape. Predictions so obtained agree well with experimental data, at atmospheric and higher pressures.

Steam bubble formation due to evaporation at the bubble wall has has been studied using ITM with phase change. Good agreement with measured data and results of analytical modelling has been observed, as shown in Figure 9-1.

Figure 9-1: Bubble growth due to evaporation at the bubble-curved surface: comparison between analytical, CFD and experimental growth curves.
The simulation of bubble formation in high-pressure conditions was found to be affected by numerically generated spurious currents. Two methods have been tested, capable of reducing considerably the currents (Giustini, Murallidharan et al. (2015)).

The prediction of bubble growth was found to be weakly affected by the spurious currents, even though such currents had a macroscopic influence on the details of the liquid flow close to the bubble-curved surface.

9.1.2 Microlayer evaporation and the fundamentals of the evaporation process

Evaporative thermal resistance is generally not included in microscopic modelling of vapour bubble growth. However, it has been shown in this work to be important in some circumstances, and in particular in the understanding of the evaporation of the microlayer beneath the bubble (Giustini, Jung et al. (2016)). For many conditions, microlayer evaporation is a significant contributor to the vapour forming the bubble. The flow of heat through this layer has been shown to be strongly affected by the evaporative ‘heat transfer coefficient’.

This has been demonstrated by analysis of a recent set of experiments, where the inclusion of this phenomenon is clearly shown to be able to restore consistency to the heat flux derived from two otherwise mutually self-consistent independent measurements, as shown in Figure 9-2. Evidence has been gathered that the cause of this odd behaviour is most likely associated to the molecular mechanism of evaporation. A model of microlayer evaporation, based on kinetic theory, was able to produce results that are in good agreement with measured data, if the hypothesis of ‘partial sticking’ of vapour molecules impinging on the microlayer surface is introduced. Similar suggestions have been advanced by previous analyses in different contexts, and the present numerical results are in broad consistency with these.
Figure 9-2: Evidence of partial sticking of vapour molecules impinging on a liquid surface, deduced from observations of microlayer depletion.

This phenomenon, of ‘imperfect evaporation’ of the microlayer has been incorporated in the microlayer sub-model of the interface tracking code PSI-BOIL. The influence of this phenomenon on computed bubble growth has been clearly demonstrated for the case of water at atmospheric pressure, as shown in Figure 9-3.

Figure 9-3: Effect of evaporative thermal resistance on computed bubble formation.
This improved understanding of microlayer evaporation, and of the role played by it in bubble growth, should allow more accurate future modelling.

9.1.3 Nucleate boiling heat transfer; the ‘quench’ component

The results presented show that the interface tracking approach with phase change is able to provide insight on fundamental aspects of the boiling process. Among the findings of this work is an assessment of the transient conduction component of nucleate boiling heat transfer, generally termed ‘quench’ in component scale heat flux partitioning (‘RPI’) modelling. This assessment indicates that the usual models employed for the quenching component give a significant overestimate of the heat so transferred. An example of such imperfect representation is shown in Figure 9-4, where the RPI quench energy transfer, and that extracted from the mechanistic simulation, are compared, showing a large discrepancy. Whilst it is a (helpful) characteristic of RPI modelling that the approach tends to cause errors in one of the components to be automatically compensated for by others, it is nonetheless obviously desirable that individual models be as accurate as possible, and that the need for tuning be minimised. Whilst of themselves the single bubble microscopic studies performed in this work cannot be used for industrial application, one of the main motivations in performing them is to provide just this kind of detailed insight and quantification, augmenting the experimental measurements on which component scale modelling has hitherto relied alone.
Figure 9-4: The large difference between the quenching energy transfer from mechanistic simulation and that computed by the RPI model.

9.2 Recommendations for future work

There are aspects where further research is plainly required.
(i) From a practical point of view, perhaps the main issue to be addressed by future investigations regards the computational cost of direct numerical simulations of boiling phenomena, which needs to be reduced, either via adopting adaptive meshing techniques, or via changing the approach to modelling evaporation at the liquid-vapour interface.

(ii) The encouraging results of an embryonic investigation of the vaporization mechanism here shown indicate that the sophisticated experimental techniques developed to study bubble growth provide an exciting possibility to broaden their scope into this more fundamental investigation of the evaporative process. In particular, this can exploit the unusual circumstances where a growing bubble, under some conditions, causes a very thin liquid layer to be formed and to evaporate, providing conditions under which the evaporative process itself plays a major role in the overall heat and mass transfer.

(iii) This improved representation of the vaporization process has been included here in the microlayer modelling, and has been applied to water, but there is a wide range of fluids and conditions where further study could be beneficial.
REFERENCES


