

Growth and Departure Dynamics of Isolated Vapour Bubbles: An Improved CFD Model for Bubble Evolution in Pool Boiling

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Abstract

An improved CFD model is developed and evaluated to be used as a mechanistic model for bubble inception, growth and departure mechanism by accounting for wide range of parameters and acting forces. Critical deficiencies of earlier CFD models are recognised, discussed and alternative schemes are suggested. Well-trusted bulk empirical models are used for a limited examination and validation of model whilst heating intensity varies and satisfactory agreement supported accurate qualitative post-processing of bubble evolution in pool boiling.

Introduction

In boiling of liquids, the growth and detachment of vapour bubbles critically determine the characteristics of boiling regimes, and the rates of heat and mass transfer. The dynamics of vapour bubbles essentially dependant on interactive forces of flow inertia, surface tension and buoyancy. Influence these complex forces and their relative strength regulates the bubble growth rate, bubble shape and departure frequency. Even with carefully-planned sophisticated experimentation [1], the interdependency of boiling parameters makes it virtually impossible to separate and examine the specific influences of individual flow parameters on bubble dynamics. Such difficulties in experimental evaluation of bubble life-cycle during boiling process promotes the necessity of numerical approaches which allow refining the spatial and time scale of the investigation.

Developing numerical simulation of pool boiling, in either time-resolved or averaged schemes, involves a wide range of time and spatial scales variation where domain dimensions (0.1-10 m) are not comparable with boiling critical dimensions such as bubble and cavity radius (1-100 μm). One of the common solutions for such fluid dynamics fundamental barrier is to determine and introduce micro-scale parameters as scalars correlated with macro-scale field parameters. This implementation method is the key basis of recent boiling analytical and CFD models. In the process of the field development, improved computational abilities have allowed researchers to be more ambitious toward resolving phenomena rather than modelling them; yet, fully resolved approaches cannot be considered as a feasible and cost-effective options due to massive computational demand for information which hardly could be validated against experimental measurements. Moving toward fully mechanistic modelling of such intricate phenomena begins from a better investigation of bubble growth, departure and mutual field influence. With reference of well-trusted literatures, accounting for single parameter, this paper addresses a generic modelling approach and validation to assure reliability and versatility of a CFD framework in presence of surface tension, wall adhesion, and thermal boundary layer in various operating conditions.

Bubble departure diameter and frequency are strictly dependent parameters that could be affected by complicated interactions

between surface tension, buoyancy, inertial and wall adhesion forces. Literature of the field includes investigations led to correlating these parameters with certain field scalar. Fritz [2] observes process of bubble departure for fields of air bubble in water and vapour bubble in water, mercury and Carbon tetrachloride with combinations of operating conditions. He concludes, for reported conditions (moderate pressure change), wall contact, surface tension and buoyancy forces are determining terms, and on such basis correlates Bond number (

$B_o = \frac{g(\rho_l - \rho_g)D_d^2}{\sigma}$) by contact angle. The Ruckenstein model

[3] correlates Bond number with Jacob number representing influence of heating intensity provided to boiling field. Such dependency is also confirmed by Zuber's investigation [4] which proposes bubble Bond number as function of wall superheat. Cole and Shulman [5] investigated bubble growth process in high Jakob number and suggested a correlation for Bond number at departure threshold accounting for operating pressure independently. Their experiment was carried out using water, Methanol and n-Pentane for atmospheric and sub-atmospheric conditions, and provided strong validation for their suggested correlation whilst heat flux and surface characteristics remain unchanged. Introducing a comprehensive and versatile CFD model, as a mechanistic approach, these closures are used as experimental benchmarks to assess influence of wall heating, on bubble departure diameter. Critical forces may be investigated with reference of bubble shape and deformation during growth and at departure threshold as a qualitative description of the cycle.

In addition to bubble departure size, it is crucial to calculate time scale of growth process, determining required time for a single bubble departure. That would be matter of interest for heat transfer analysis on the surface (growth time) and mass transfer due to nucleation in the flow field (departure frequency). Bubble cycle, during boiling process, includes a dwelling (waiting) period before growth process triggers. Hence, for estimation of release frequency both dwelling and growth times should be accounted. Current work suggests a simple, yet consistent closure for estimation of dwelling time and compares it with former models before benchmarking the final parameter of bubble departure frequency. Bubble departure frequency, in the pool boiling case, has been extensively investigated in last decades and many correlations are suggested for various operating conditions. Among which, this study indicates, closures suggested by Jakob [6], Zuber [7], and Cole [8] as simple, yet, well-trusted and widely tested for pool boiling. Jakob [6] proposes that product of bubble departure diameter and frequency as a constant and later Zuber [7] extends that model by accounting for Bond number. Cole's experiment [8] confirms such physics, and brings additional effect of bubble drag coefficient into account led to new correlation between bubble release frequency and Bond number. In establishing a generic

approach to evaluate bubble mechanistic model it is critical to be consistent with range of applicability as a certain correlation is applied for comparison purposes.

In improving drawbacks in former CFD models, which have investigated bubble growth and departure phenomena, this paper has three major numerical objectives. That includes novel assumption to appropriately consider phase change process, initial field conditions and dwelling time approximation.

Numerical method

The model is to be used for prediction of bubble departure diameter and frequency governed by interaction of various forces in a very small time fraction whilst the bubble is growing. The bubble grow rate is controlled by rate of mass transfer due to evaporation (at nucleation site and interfacial area) and condensation. Since flow, in pool boiling, is solely buoyancy induced, coupled momentum and mass transfer has a significant influence on force regimes. That means unrealistic mass transfer term, not only does impose incorrect bubble growth rate, but also originates inaccurate inertial force leading to wrong bubble shape, force interaction regime and ultimately wrong departure features. Hence, the improvement is required to overcome common drawbacks recognised in bubble departure modelling. The most prominent drawbacks from literature could be briefed to undermining influence of initial boundary layer development and defining constant mass transfer coefficient, independent of bubble shape and growth rate.

Multi-phase model

Set of equation to account for mass, momentum and energy conservation of each phase, coupled by phase exchange terms, form the multi-phase model. VOF is the most common and cost-effective approach for phase tracking which has been widely used and validated for liquid-gas applications. For unsteady, laminar, liquid-vapour field, continuity equation, for liquid phase, is written as:

$$\frac{\partial}{\partial t}(\alpha_l \rho_l) + \nabla \cdot (\alpha_l \rho_l \vec{U}_v) = \dot{m}_{vl} - \dot{m}_{lv} \quad (1)$$

Where is α volume fraction, and $\dot{m}_{vl}, \dot{m}_{lv}$ represent rates of condensation and evaporation, and the same equation could be developed for vapour phase. For accurate interface capturing, appropriate interpolation technique near the interface (zero-one volume fraction values) is to be utilised. Obtaining volume fraction value is a key step in VOF assisting to calculate phase average material properties, and hence energy equation is shared between phases. Single VOF momentum equation for the entire domain would be

$$\frac{\partial}{\partial t}(\rho \vec{U}) + \nabla \cdot (\rho \vec{U} \vec{U}) = -\nabla p + \mu \nabla^2 \vec{U} + \rho \vec{g} + \vec{F} \quad (2)$$

Velocity and material properties, in eq.2, are phased averaged and where term $\rho \vec{g}$ is responsible for buoyancy force and \vec{F} includes surface tension and wall adhesion forces with consistence form and dimension. Phased averaged form of energy equation used in VOF scheme is then as:

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{U}(\rho E + p)) = -\nabla \cdot (k \nabla T) + S_h \quad (3)$$

S_h source term includes impact of phase change in energy equation (i.e. $S_h = -\dot{m}_{lv} h_{lv}$) and k is phase averaged thermal conductivity.

Interfacial forces and phase exchange schemes

Surface tension and wall adhesion forces are implemented by use of Brackbill et al. [9] model which is simple and accurate; yet, could be problematic, due to sharp interfaces, if solver requirements are not considered appropriately. In presence of mass transfer, sharp interface numerical treatments such as Level set function are inapplicable and appropriate solver and interpolation method are to be chosen avoiding unrealistic diffusive interfaces.

Interfacial mass transfer, as discussed, is a key parameter determining growth rate and shape. Lee [10] model is a mechanistic model based on Hertz-Knudsen estimation of mass flux near saturation point. Hertz-Knudsen [11,12] equation proposes interfacial mass flux ($kg/m^2.s$) value in term of operating and saturated pressure. Incorporating Clapeyron-Clausius equation interfacial mass flux equation could be rewritten as:

$$\Gamma = \beta \sqrt{\frac{M}{2\pi R T_{sat}}} \frac{h_{lv}}{(1/\rho_v - 1/\rho_l)} \left| \frac{T - T_{sat}}{T_{sat}} \right| \quad (4)$$

Equation.4 could be used for evaporation or condensation where M , R and h_{lv} are molecular mass, universal gas constant and latent heat respectively. Parameter β , known as accommodation coefficient, assumed as 1 near equilibrium condition. Hence, Local mass transfer is

$$\dot{m}_{lv} = -\dot{m}_{vl} = \Gamma I_{AC} \quad (5)$$

where I_{AC} is interfacial area concentration. Lee model substitute all the constant terms in mass flux equation alongside with assumption of constant area concentration and defines evaporation/condensation coefficient for a certain operating condition. Assumption of constant area concentration could be acceptable for time averaged models where the time (and correspondingly dimension) scale is larger than bubble evolution time (and diameter) scale [13]. Assuming interfacial area concentration and accordingly mass transfer rate as a uniform (space-wise) and constant (time-wise) parameter is an absolutely unacceptable assumption for a bubble growth and departure model. Briefing disadvantages of such model, first, bubble growth (and departure) rate will be severely and unrealistically dependent on the proposed constant. Then, unrealistic mass transfer rate will induce additional momentum source, resulting in factitious inertial forces. The combined effect will misinterpret governing forces, bubble shape and departure threshold. Improving the deficiency, current model calculates the precise value mass transfer rate, by calculating local interfacial area concentration as

$$\dot{m}_{lv} = -\dot{m}_{vl} = \Gamma \left| \nabla \cdot \alpha \right| \quad (6)$$

That completes the scheme for evaporation and condensation as interfacial mass transfer phenomena. However, boiling includes another source of mass transfer which takes place at the solid-fluid surface and is critically determined by micro-scale imperfections known as cavities.

Cavity model

Accounting for cavity role in boiling process is a critical issue as bubble initially incepts inside cavity and later there will be a periodic influence from cavity on boiling characteristics. Current model accounts for cavity characteristics (e.g. shape, volume and mouth area) to essentially deliver critical parameters into CFD model. Two stages are proposed here before the entire cavity liquid mass is vaporised and bubble interface reaches to the

cavity mouth. The first stage is to heat up the cavity liquid from bulk to saturated temperature. The associated time is calculated as:

$$t_{DA} = \frac{Q_{req}}{\dot{Q}_{cavity}} = \frac{\rho_l V_{cavity} c_{pl} (T_{sat} - T_l)}{\dot{q}_{total} A_{cavity}} \quad (7)$$

To calculate volume and surface area of cavity, dimension and shape of which are to be assumed. The second stage represents the time required for evaporation of the cavity liquid content:

$$t_{DB} = \frac{\int_0^{t_{DB}} m_{cavity} - \dot{m}_{cavity} dt}{\dot{m}_{cavity}} = \frac{h_{lv} \rho_l V_{cavity}}{2 \dot{q}_{total} A_{cavity}} \quad (8)$$

The total dwelling time scale consists of these two components (i.e. $t_D = t_{DA} + t_{DB}$). Besides, there will be no mass transfer due to evaporation/condensation as far as no interfacial area is introduced to the domain. Highlighting a novel feature of current phase change model, even in superheated liquid phase change does not occur unless a non-zero volume fraction gradient (representing bubble-liquid interface) is induced. This is a well-understood boiling physics which is not seen in most of boiling numerical models and here is accounted by incorporating cavity dimensions.

Dwelling time is also important for thermal diffusion before nucleation process and determines the thermal boundary layer characteristics, influencing bubble growth.

Domain and boundary conditions

Computational domain is a 2D rectangular box with height (+y) of 250 mm and width of (+x) 100 mm to be solved in an axisymmetric framework. Having domain meshed with uniform grid spacing of 10 μm , cavity mouth could be captured with reasonable resolution reducing chance of numerical instability. Such grid refinement increases computational demand, not only directly by number of cells, but also indirectly by need of time step refinements. Axis boundary is the right-sided edge and assuming gravity downward (-y), below wall represents nucleation site where cavity and heated surface are located. The small segment (0.5 mm) of below wall, next to axis boundary, represents heated surface surrounding the central cavity (50 μm). Another vertical edge opposite to the axis boundary is defined as wall, well away from nucleation site to minimize shear effect. The boundary at topside of domain is set to be pressure outlet at operating pressure. Thermal boundary condition at all wall, except the heated wall, is isothermal boundary condition at the bulk temperature (373 K) where the saturated temperature is set with respect to operating pressure (373.15 K @ atmospheric). The heated surface is a constant temperature boundary superheat with Jakob number reference.

Solver

Using shared-field approximation (for velocity, energy and material properties) increases the chance of numerical instability and divergence, particularly for cases with high ratio of phases' material properties (e.g. density ratio > 750). This common problem is discussed in literature and combination of velocity-pressure decoupling method, discretisation schemes and under relaxation factors are proposed for various bubble growth cases. Nevertheless, current mass transfer scheme is being applied with no previous records and indicates a sever sensitivity against solver method, relaxation factors and time marching. Briefing the solver setup, a coupled solver is used with PISO scheme for pressure-velocity decoupling and Geo-Reconstruction interpolation for volume fraction.

Setup and computational stages

Two stages are marked as essential computational steps to incorporate cavity and dynamic mass transfer closures. Acknowledging the physical fact that nucleation does not incept unless the thermal boundary layer is developed, after initializing the fluid domain with bulk temperature, it should be given a sufficient time to develop thermal boundary layer under diffusive-buoyancy scheme. At this stage domain simulate condition where bubble interface expands out of the cavity. Working out dwelling time from eq.7&8, void fraction of one is manually assigned to first cell row on top of cavity to simulate cavity bubble inception effect. This obviously requires assuming size of cavity mouth which here assumed as 50 μm . A superheated temperature field with non-zero interfacial area concentration will trigger mass transfer from this point. Self adjusted mass transfer coefficient, determined by degree of superheat, shape and dimension of the bubble, is expected to be more realistic. Hertz-Knudsen equation is just applicable for flat surfaces; the requirement that is well respected here since calculation of interfacial area is carried out on cell basis as sufficiently small dimension.

Time step refinement is crucial requirement to maintain numerical stability and obtain convergence and is basically estimated by a Courant number requirement. Such time step may be refined further by restrictions due to surface tension, gravity and viscous forces. For the current model refinement due to

surface tension force ($\Delta t_\sigma \approx \sqrt{\frac{(\rho_l + \rho_g) V_{cell}}{4\pi\sigma}}$) is the finest and critical to be applied.

Results and validation

A brief set of results are represented to highlight novel findings, validations and essential modelling components.

Thermal boundary layer and Dwelling time

Bubble evolution cycle takes place within a small time scale which is fraction of time required for thermal boundary layer (TBL) development. A superheated liquid layer (SLL), which is formed at the lower section of TBL, plays a critical role in bubble formation. Not only growth rate does depend on thickness of SLL, shape of bubble is majorly affected by this layer. Development of TBL is initially determined by diffusion mechanism and by increasing wall Jakob number (

$$Ja_w = \frac{\rho_l C_{pl} (T_w - T_{sat})}{\rho_g h_{lv}}$$

), contribution of buoyancy terms will be more considerable. Although, growth of TBL and SLL is part of numerical simulation, it is crucial to impose right initial condition once the bubble interface reaches to cavity mouth.

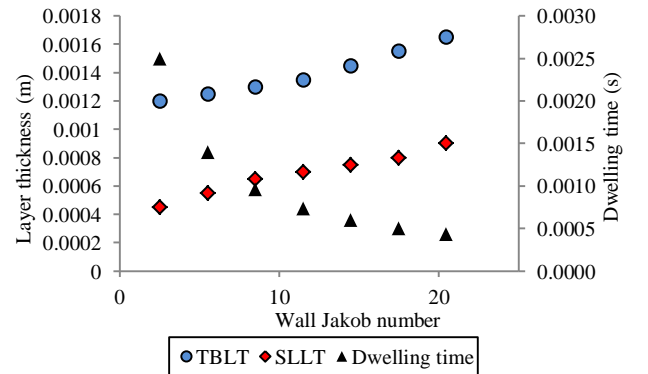


Figure 1. Dwelling time, thermal boundary layer (TBL) and superheat liquid layer (SLL) thickness (Accuracy = 50 μm)

As demonstrated in figure.1, more heating reduces dwelling time and increases thickness of both TBL and SLL. Therefore, it could be briefed that, at high Jakob number, contribution of dwelling time in bubble evolution cycle is less and interfacial mass transfer is dominating mechanism for bubble growth, due to higher SLL thickness.

Growth time and departure frequency

Growth process is the section of bubble evolution which determines shape and diameter of departing bubble and associated frequency. Simplified mass transfer schemes, with constant evaporation-condensation coefficient, are found inappropriate for bubble evolution modelling since they consider a constant interfacial area to calculate the mass transfer coefficient. Therefore, bubble departure diameter (and correspondingly growth time) cannot be considered as independent simulated parameters and are indirect model's input. Shape and diameter of departing bubbles are considered as criteria to investigate interaction between forces where inertial forces are associated with mass transfer rate. Bubble departure frequency is additional measure for evaluation of bubble growth rate. Figure.2 compares bubble shape at three Jakob numbers for a saturated boiling case (i.e. $\Delta T_{\text{sub}}=0.15$ K).

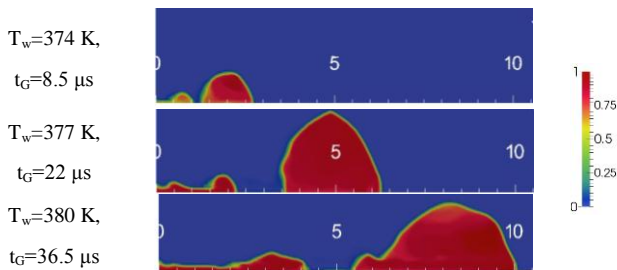


Figure 2. Vapour volume fraction at departure threshold; representing vapour plume and separated bubble for saturated boiling; Axisymmetric representation - gravity is directed left

Empirical departure diameter models, which account for wall heating effect [3,4], have not considered influence of sub-cooling as a direct parameter. Hence, the investigation is initially set for a very low sub-cooling degree to minimize effect of sub-cooling. Initially developed superheat layer extends the area at which interfacial evaporation takes place and hereafter vapour plume and is extended and bubbles obtain an elongated shape at departure threshold.

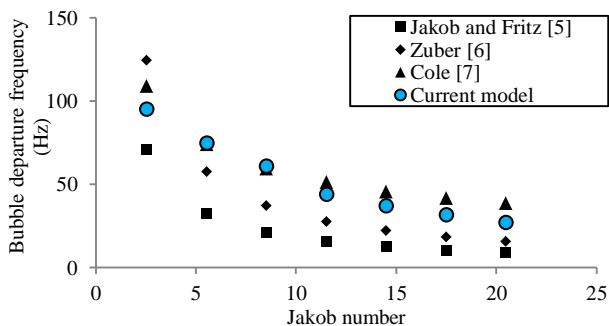


Figure 3. Comparison of bubble departure frequency with empirical closures

Departure diameter is evaluated against Ruckenstein [3] and Zuber [4] model and found reasonably matched, taking the fact into account that some of operating parameters from experimental condition remain unexplained. Figure.3 compares departure frequency with three empirical models [6,7,8] where departure frequency calculated by current CFD model obtains the

same variation trend as other empirical models and suggested values are within the range of other model's variation. All the benchmark models, suggested for departure frequency, have a dependency on departure diameter. Therefore, comparison depicted in figure.3 could be deemed as growth rate validation and indirect evaluation of departure diameter, in addition to earlier comparison with Ruckenstein and Zuber models.

Conclusions

CFD approach for bubble evolution is improved by modification of mass transfer scheme, initial condition (initial thermal boundary layer thickness is accounted) and suggesting a new simple model for dwelling time (departure frequency is modified for low wall heating). Results are evaluated against bulk empirical models and appropriate level of matching is obtained. The proposed CFD framework is a mechanistic model, competent to account for contact angle, surface tension, thermal boundary layer development and growth. Therefore, it is more general analysis approach and preferred to those bulk models, usually accounting for limited parameters and limited range applicability.

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