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Abstract

To improve the closure relations employed for component-scale Computational Fluid Dynamics simulation of boiling flows, a first-principles method for predicting bubble departure diameters in flow boiling has been developed. The proposed method uses minimisation of the free energy of a system in thermodynamic equilibrium to predict the contact angle and the resistance to sliding of a vapour bubble attached to a surface in the presence of a forced liquid flow. Predictions of the new method are compared with measurements from existing experimental databases, and agreement with data is shown to be comparable or superior to that obtained with previous bubble departure models that have generally used a force-balance approach. The main advantages of the energy-based method over the previous force-based methods are that its formulation is simpler, and that the new model does not require the use of ad hoc tunable parameters to define force terms, or geometrical characteristics of the attached bubble such as its base area, which cannot be confirmed experimentally. This increases confidence in the validity of the new approach when applied outside the rather limited range of current test data on bubble departure in flow boiling.

Keywords	boiling heat transfer; bubble departure; flow boiling

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Submission Files Included in this PDF

File Name [File Type]

Bubble_departure_cover_letter.docx [Cover Letter]

Bubble_departure_response.docx [Response to Reviewers]

Bubble_departure_highlights.docx [Highlights]

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"Modelling of bubble departure in flow boiling using equilibrium thermodynamics"

Dear Professor Rose,

The attached response to the reviews of the manuscript "Modelling of bubble departure in flow boiling using equilibrium thermodynamics" is submitted for your consideration.

Enclosed are:

- A point-by-point response to the Reviewers' comments

- A revised manuscript.

In the response, original comments are coloured in blue, and our responses are coloured in black. In the revised manuscript, additional text is highlighted in yellow. Any additional figure appearing in the revised manuscript has been referenced in the response.

I hope that the rebuttal will help to clarify the doubts expressed by the reviewers' requests, and look forward to hearing from you.

Yours sincerely

Giovanni Giustini

Response to the Reviewers' comments

Reviewer #1

'The use of free energy minimization to establish the point at which equilibrium is disturbed gives the same result as a force balance to identify when equilibrium is disturbed. In reality, only a quasi-equilibrium state ever exists since bubble growth is very rapid, and the bubble shape (assumed uniform) is constantly evolving. It appears to be over-stretching to claim a more rigorous bubble detachment criterion.

The claim of a first principles model is also a stretch. The contact region is modeled, and there is no verification that the model presented is better than any other model. Nor does experimental verification exist for the entire contact region.'

The authors thank the Reviewer for these helpful comments.

The authors consider that the energy-based method does have some advantages over the force balance approach and does not always give the same result as the latter. In particular the ability to predict the contact area between the bubble and the heated wall is seen as a positive aspect. The first bullet point in Section 6 of the paper has been reworded to make that point more clearly.

The authors agree with the reviewer that experimental verification of the prediction of the bubble base contact area is somewhat lacking, but do not agree that it is completely non-existent. Figure 14 in Ref [11] of the revised submission shows that the energy-based method gives reasonable agreement with experimental measurements of the time varying base contact angle during bubble growth in atmospheric pressure pool boiling at two effective gravity levels, implying that the transient base area is calculated reasonably accurately by the model.

The authors agree that only a quasi-equilibrium condition can exist as the bubble is growing very quickly. Faithful representation of the bubble shape is feasible strictly only by using Computational Fluid Dynamics (CFD) methods that employ Interface Capturing techniques. However, these methods are not yet reliable for quantitative studies and in addition are not yet feasible for large-scale simulation campaigns due to excessive computational cost. Given the unavailability of a practical CFD method, the energy minimisation method, which treats the attached bubble as a truncated sphere that is always in a state of thermodynamic equilibrium, seems to provide a good compromise between simplicity and accuracy.

To summarise, although it is conceded that the model is imperfect and - just like all extant models – can return only approximate estimates of bubble departure diameters, it nonetheless is seen to have some advantages over previous methods.

'In comparing models, the most recent models are not used. For example,

Thorncroft, G.E., Klausner, J.F., and Mei, R., "Bubble Forces and Detachment Models," *Multiphase Science and Technology*, Vol. 13, Nos. 3 & 4, pp. 35-76 2001.
supercedes all other bubble detachment models presented by the Thorncroft et al., but no mention of this paper is made. It is relevant because it attempts a more rigorous approach to the detachment criterion.'

We thank the Reviewer for this helpful comment. The suggested reference has been acknowledged in the text.
Predictions obtained with the 2001, augmented model by Thorncroft et al have been analysed, but do not appear significantly different numerically from those of the earlier models by Klausner and Zeng, cited in the text.
The refined model of Thorncroft can indeed be considered more rigorous than the earlier models of Klausner and Zeng. However, like its earlier versions, it has the drawback of not providing a means for computing the bubble base contact area, which is considered as a free input parameter. On the other hand, as discussed above, the energy-based model provides a computation of the bubble base contact area as a result of use of the free energy minimization equation.

Reviewer #2

'(1) Figure 1 should show the advancing and receding contact angles separately, rather than shown one angle "theta" at both advancing and receding positions.'

We thank the Reviewer for this helpful comment. Figure one has been modified accordingly.

'(2) The definition of surface inclination angle in this manuscript is the opposite to that in the reference [22] (Sugrue et al. 2014). Is the experimental data shown in Figure 4 for upward or downward facing horizontal?'

The current definition of the inclination angle indeed respects a different convention than the one adopted by Sugrue et al. In figure 4, experimental data is shown for a downward facing horizontal surface, as are predictions of the model. In the caption, text has been added clarifying the orientation of the surface.

(2, continued) 'In addition, Figures 4 , 5 and 6 do not show all the detailed control parameters such as heat flux and subcooling.'

We thank the reviewer for this helpful comment. Omitting these control parameters might indeed have been a source of confusion. In new captions of figures 4, 5 and 6, all the relevant control parameters have been clearly stated. (We have chosen to specify the parameters in the caption lest the figures become crowded with text).

'(3) The contact angle hysteresis parameter in Figure 8 does not show clear indication that the choice of 0.07 is the best fitting value. More attempting of this parameter is recommended to improve figure 8.'

We thank the Reviewer for this helpful comment.

Bubble departure diameters have been recalculated for all test cases considering a value of $\varepsilon = 0.105$, in order to ascertain the existence of a minimum of the error of predicted departure diameters in the range between $\varepsilon = 0.07$ and $\varepsilon = 0.14$.
We also appreciate that the original figure is unclear due to crowding of lines. We have replaced the original figure with a new figure showing comparison between RMS errors of the present model (as a function of the contact angle hysteresis parameter),

and of the other models that have been considered, including results with the previously unexplored case of $\varepsilon = 0.105$.
The new results confirm that, for $\varepsilon = 0.07$, the root mean square error of predicted bubble departure diameters is at a minimum.

Highlights

- First-principles model of steam bubble departure in forced flow boiling
- Application of model to well-established experimental data sets
- Assessment via comparison with existing models
- Deficiencies of existing models are highlighted, and eliminated by proposed model.

Modelling of bubble departure in flow boiling using equilibrium thermodynamics

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Abstract

To improve the closure relations employed for component-scale Computational Fluid Dynamics simulation of boiling flows, a first-principles method for predicting bubble departure diameters in flow boiling has been developed. The proposed method uses minimisation of the free energy of a system in thermodynamic equilibrium to predict the contact angle and the resistance to sliding of a vapour bubble attached to a surface in the presence of a forced liquid flow. Predictions of the new method are compared with measurements from existing experimental databases, and agreement with data is shown to be comparable or superior to that obtained with previous bubble departure models that have generally used a force-balance approach. The main advantages of the energy-based method over the previous force-based methods are that its formulation is simpler, and that the new model does not require the use of *ad hoc* tunable parameters to define force terms, or geometrical characteristics of the attached bubble such as its base area, which cannot be confirmed experimentally. This increases confidence in the validity of the new approach when applied outside the rather limited range of current test data on bubble departure in flow boiling.

1 INTRODUCTION

Numerical simulations of boiling flows using phase-averaged Computational Fluid Dynamics (CFD) methods rely on sub-models of the wall-boiling process to describe the 'heat flux partitioning' between evaporation and single-phase heat transfer to the liquid [1] [2] [3]. Such models are sensitive to the assumed diameter of bubbles at the point of departure from a nucleation site [4], which must be calculated using separate sub-models. The accuracy of these bubble departure models ultimately determines the accuracy of a CFD simulation that uses heat-flux partitioning.

A number of empirical and semi-mechanistic methods have been developed in the past for predicting bubble departure diameters in flow boiling. Most of these use a force-balance approach originally proposed by Klausner et al. [5], who identified the point of bubble departure with the condition that the net force on the bubble due to buoyancy, surface tension and fluid drag and lift, in the direction either parallel or perpendicular to the surface, was equal to zero. Examples of force-balance models can be found in Refs. [6], [7], [8], [9] and [10].

The force-balance approach has the significant disadvantage that it provides no means of determining the contact area between the bubble and the heated surface at the point of departure. This is a crucial omission since the contact area determines the magnitude of the wall adhesion force due to surface tension that resists departure. To determine the adhesion force, current force-balance models generally treat the bubble base area as an unknown parameter that is adjusted to fit the experimentally measured departure diameters. However, the absence of a method for determining *a priori* the bubble base contact area leads to concern that such models may give misleading results if applied outside the range of available databases, which generally exclude the industrially important case of high pressure boiling.

In a recent study [11], we used equilibrium thermodynamics to develop a first-principles method for predicting bubble growth and departure diameters in pool boiling, which used minimisation of free energy to find the time-dependent contact angle at the base of a growing bubble, and hence its base contact area. The method was shown to give reasonable agreement with departure diameters measured in pool boiling experiments for a broad range of fluids and pressures, but its applicability was limited to bubble departure in boiling on horizontal upward facing surfaces in the absence of any imposed flow.

In this paper, the Ref. [11] model is extended to the case of flow boiling on an inclined surface, in which bubble departure may be by sliding along the surface as well as by lift off. The extended model is validated against measurements of bubble departure diameter in flow boiling in a variety of fluids, and for various degrees of subcooling, fluid velocity, and surface inclination.

The paper is structured as follows. The extension of the Ref. [11] bubble departure model to include an imposed liquid flow and an inclined surface is described in Section 2. Section 3 analyses the existing experimental database to establish an optimum value for the difference between the advancing and receding contact angles, for use as input data to the model. Section 4 demonstrates the capability of the model to capture experimental trends with flow velocity, inclination and pressure, and Section 5 compares the current model with existing models for predicting bubble departure. Finally, discussion and conclusions are provided in Section 6.

2 MODEL OF BUBBLE DEPARTURE

2.1 Model assumptions

In the present work, the method of Ref. [11] for predicting the time evolution of the contact angle during bubble growth in horizontal pool boiling, is extended to the case of forced convective boiling on an inclined surface. As before, the fundamental assumption is made that an attached bubble is always in a state of thermodynamic equilibrium under the forces that it instantaneously experiences. Figure 1 shows the assumed physical representation of the growing bubble and the forces acting on it.

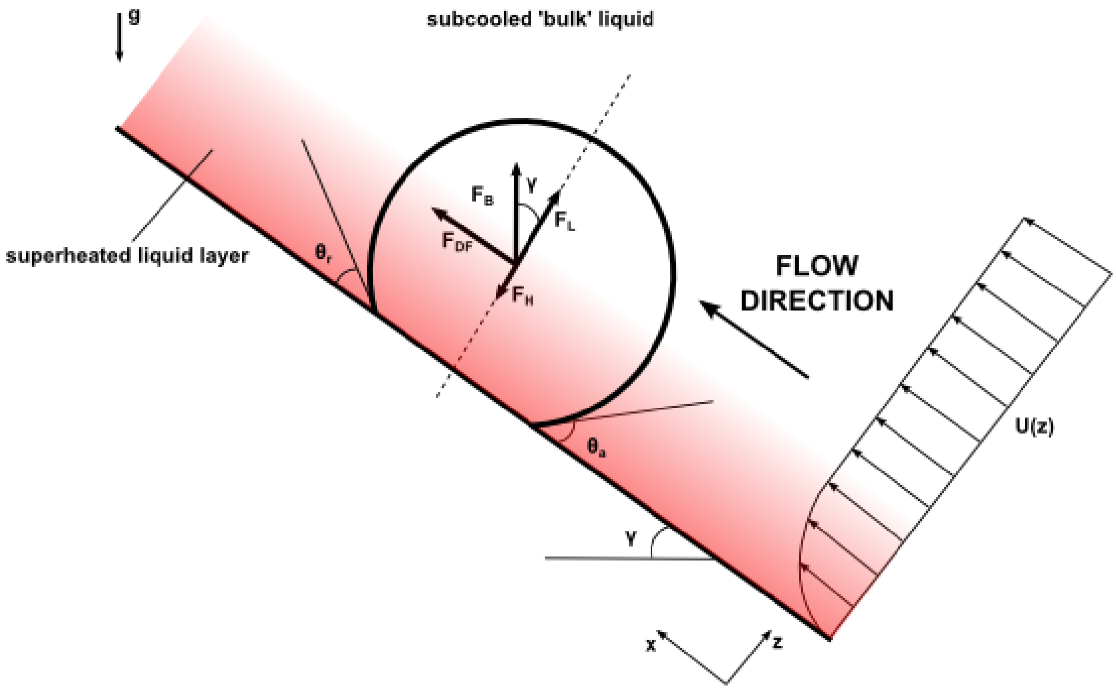

Figure 1
System considered: a steam bubble growing at a heated surface into subcooled fluid flowing tangential to the surface.

The main assumptions of the model are as follows:

1. The bubble is assumed to be growing at an active nucleation site on an inclined heated surface in the presence of a forced flow of subcooled or saturated liquid. A layer of superheated liquid is assumed to exist adjacent to the heated surface, beyond which the liquid temperature decreases to the bulk liquid temperature. The bubble is assumed to grow due to formation of vapour by evaporation from its surface.
2. Referring to Figure 1, the external forces acting on the bubble are assumed to be (i) a buoyancy force $\boldsymbol{F}_B$ that acts vertically upward, (ii) a hydrodynamic reaction force $\boldsymbol{F}_H$ due to bubble radial growth that acts in the negative *z* direction, (iii) a lift

force $\boldsymbol{F}_L$ due to the liquid velocity gradient close to the surface, that acts in the positive *z* direction and (iv) a fluid drag force $\boldsymbol{F}_{DF}$ due to the imposed liquid flow that acts in the positive *x* direction.

3. The bubble is assumed to always approximate to the shape of a spherical cap with a unique radius of curvature *R* and unique base contact angle θ, both of which are assumed to vary with time. In the presence of an imposed flow and/or surface inclination, θ is expected to vary slightly around the base of the bubble due to the action of buoyancy and fluid forces: in forming the equation for θ this variation is neglected, so the value of θ calculated is to be regarded as an average value around the bubble base.
4. It is assumed that bubble detachment from the nucleation site can occur by lifting off from the surface or by sliding along it. Bubble lift-off is identified as the point at which the base contact angle θ falls to zero, as in the earlier model [11]. Bubble sliding is identified with the point at which the bubble becomes unstable against a small displacement in positive *x* direction, resulting in unconstrained motion along the surface. The bubble diameter at the point of detachment from the nucleation site, irrespective of whether it is by lift-off or sliding, is termed the 'departure diameter'.
5. As in the earlier model [11], the temperature of the vapour inside the bubble is assumed to be uniform and equal to the saturation temperature at the externally imposed pressure. The vapour in the bubble is assumed always to be in thermal equilibrium with the liquid at the bubble curved surface [12].
6. Also as in [11], spatial variations of the pressure inside the bubble, due to fluid dynamic and hydrostatic forces, are assumed negligible, as in the classic theory of Plesset [13]. Pressure variations in the liquid at the bubble wall due to the hydrodynamic and hydrostatic forces are taken into account in the model.

2.2 <u>Equation for dynamic contact angle</u>

2.2.1 Summary of Ref. [11] model

The Ref. [11] model calculates the contact angle θ at each point in time by using the condition $\delta\tilde{A} = 0$, where $\tilde{A}$ is the thermodynamic availability (free energy) of the system represented by the bubble and its surroundings. The change $\delta\tilde{A}$ in availability due to a small perturbation from the bubble's equilibrium shape is calculated as:

$$\delta\tilde{A} = -\delta V_B \Delta p + \sigma\delta A_S + \left(\sigma_g - \sigma_f\right)\delta A_b + \delta W_s \quad (1),$$

where V_B is the bubble volume, Δp is the pressure difference between the vapour inside the bubble and the ambient pressure, σ is the surface tension coefficient of the liquid-vapour interface, A_S is the area of the bubble curved surface, σ_f and σ_g are, respectively, the surface energies per unit area of the liquid-solid and vapour-solid interfaces, and A_b is the bubble base area; δW_s represents the work done by hydrostatic and fluid dynamic forces acting on the surface of the bubble.

Using equation (1) and applying the condition that $\delta\tilde{A} = 0$ for perturbations in θ at constant *R* and in *R* at constant θ, the following implicit equation is derived for the base contact angle of an attached vapour bubble in horizontal pool boiling:

$$\begin{aligned} & R^{+2}\left[\frac{2}{3}\phi_1 - \frac{1}{2}\frac{\phi_2^2}{\phi_1}sin^2\theta\right] - R^{+}\dot{R}^{+2}\left[C_D\phi_2^2\phi_1^{2/3} - \frac{1}{4}\frac{\phi_2}{\phi_1}sin^2\theta\right] \\ & -\left(cos\,\theta + \frac{1}{4}\frac{sin^4\theta}{\phi_1}\right)\left(cos\,\theta - cos\,\theta^*\right) = 0 \end{aligned} \quad (2),$$

where non-dimensional variables are $R^+ = R/\left(\frac{\sigma}{\rho_f g}\right)^{1/2}$, $\dot{R}^+ = \dot{R}/\left(\frac{\sigma g}{\rho_f}\right)^{1/4}$. In these expressions, $\dot{R}$ is the growth rate of the bubble, ρ_f is the liquid density, g the gravitational acceleration of 9.81 $\mathrm{m/s^2}$, and the geometric factors ϕ_n are functions of the dynamic contact angle θ given by $\phi_1 = 0.25(-\cos^3\theta + 3cos\theta + 2), \phi_2 = 0.5(1 + cos\theta), \phi_3 = \sin^2\theta$. (In terms of these factors, the bubble height and base radius can be expressed as $2R\phi_2$ and $R\phi_3^{1/2}$, respectively). C_D is a drag coefficient for motion of the bubble in the z direction due to its radial growth, and θ^* is the thermodynamic contact angle, which is assumed to be a fundamental property of the fluid/surface system, given by the Young-Laplace equation, $\theta^* = \arccos\left[\frac{\sigma_g - \sigma_f}{\sigma}\right]$.

Ref. [11] used experimental data to infer a value of θ^* that could be applied in low pressure boiling on metallic surfaces. For high pressure boiling of water (pressures up to 50 bars), a correlation for θ^* was proposed implying that θ^* decreases with the saturation temperature, which is consistent with experimental observations and, qualitatively at least, with predictions of the surface adsorption theory of Adamson [14]. The Ref. [11] method for computing θ^* is retained in the present work.

2.2.2 Extension of model to include imposed flow and surface inclination

The Ref. [11] model was only applicable to the case of bubble departure on a horizontal surface with zero imposed flow, when the only external forces acting on the bubble are the buoyancy force and the fluid reaction force due to the bubble growth. To extend the model to forced convective boiling on an inclined surface, work done against other forces must be included in calculating $\delta\tilde{A}$: in particular the drag and lift forces due to the imposed flow, the buoyancy force component parallel to the surface, and the surface forces arising due to possible sliding motion of the bubble, must be considered. Introducing these extra force terms results in a modified equation for θ, and a new condition for stability against sliding, as described below.

2.2.2.1 Modified contact angle equation

Ref. [11] relates the work term in equation (1) to the effective z-direction forces, $\mathbf{F}_z$ and $\mathbf{F}_z^{'}$, that would be experienced by a bubble subjected to small perturbations in either θ or R. To extend the model to allow for the presence of an imposed liquid flow and a non-zero surface inclination (see Figure 1) it is necessary to modify $\mathbf{F}_z$ and $\mathbf{F}_z^{'}$ to include the lift force $\mathbf{F}_L$, and to replace the acceleration due to gravity g in the buoyancy force by its z-direction component $g\cos\gamma$. (Note that the drag force $\mathbf{F}_{DF}$ does not influence $\mathbf{F}_z$ and $\mathbf{F}_z^{'}$ as it acts only in the direction perpendicular to z.)

Assuming that the bubble remains stationary up to the point of departure, the lift force is given by the following expression [5]:

$$F_L = \frac{\pi}{2} C_L R_{EQ}^2 \rho_f \Delta U^2 \quad (3)$$

where R_{EQ} is the equivalent radius of a spherical bubble with the same volume of the actual bubble, ΔU is the velocity difference between the liquid and the stationary bubble, and C_L is a lift coefficient. ΔU is evaluated at the elevation of the bubble centroid, and is computed from a suitable time-averaged turbulent velocity profile (for the validation cases considered in the later sections of this paper, we use the universal turbulent velocity profile for internal channel flows, and the Reichardt [15] profile for turbulent Couette flow for the case of bubble growth in a liquid film - see Refs. [5, 16]). The lift coefficient is computed as in [17]:

$$C_L = 3.877 G_S^{1/2} \left[Re_B^{-2} + 0.014 G_S^2 \right]^{1/4} \quad (4)$$

where the bubble Reynolds number is defined as $Re_B = \frac{2\rho_f R_{EQ} \Delta U}{\mu}$ and G_s is estimated following Ref. [9] as $G_s = \frac{f}{8\mu} \rho_f \frac{U_b}{\Delta U} R_{EQ}$, where U_b is the bulk velocity (equal to the mass flux divided by the liquid density for internal channel flow, and, for cases of bubble growth in a film, equal to the velocity of the upper surface of the liquid film), ΔU is again the relative velocity between the liquid (its velocity being evaluated at the bubble centroid's elevation) and the (stationary) bubble, μ is the viscosity of the liquid and *f* is a friction factor. For channel flow, *f* is estimated using the standard Colebrook correlation for smooth channels. For Couette flow in a shear-driven liquid film, *f* is computed with the correlation of ref. [15].

Introducing the above changes, defining $U^+ = \Delta U / \left({}^{\sigma g}/_{\rho_f} \right)^{1/4}$ as a non-dimensional imposed flow velocity and noting that $R_{EQ} = \phi_1^{1/3} R$, the revised equation for θ in the presence of the imposed flow and surface inclination is:

$$R^{+2}\left[\frac{2}{3}\phi_1-\frac{1}{2}\frac{\phi_2^2}{\phi_1}sin^2\theta\right]cos\gamma-R^{+}\dot{R}^{+2}\left[C_D\phi_2^2\phi_1^{2/3}-\frac{1}{2}\frac{\phi_2}{\phi_1}sin^2\theta\right]+$$
$$\frac{1}{4}C_LR^{+}U^{+2}\phi_1^{2/3}\left[1-\frac{1}{2}\frac{\phi_2}{\phi_1}sin^2\theta\right]+ \qquad (5).$$
$$-\left(cos\theta+\frac{1}{4}\frac{sin^4\theta}{\phi_1}\right)\left(cos\theta-cos\theta^*\right)=0$$

2.3 Condition for equilibrium against sliding

As the bubble grows, the forces it experiences due to drag and buoyancy in the direction parallel to the surface increase. Observations [18] show that a condition can be reached in which wall adhesion forces can no longer keep the bubble pinned at the nucleation site, and the bubble departs from the nucleation site by sliding along the surface.

As in the case of lift-off, the condition for the breakdown of equilibrium by sliding can again be found by considering the change in availability $\delta\tilde{A}$ associated with a small displacement δx of the bubble from its equilibrium position. Assuming that the displacement δx involves no change in *R* or θ, equation (1) for $\delta\tilde{A}$ reduces to:

$$\delta\tilde{A}=\delta W_S=-F_{DF}\delta x-F_{Bx}\delta x+F_w\left|\delta x\right| \qquad (6),$$

where the three terms on the right hand side represent, respectively, the work done against the drag force caused by the imposed flow (F_{DF}), the work done against the buoyancy force component in the x-direction (F_{Bx}) and the work done against the wall adhesion (surface tension) force (F_w) acting along the contact line between the bubble wall and the heat transfer surface. Note that the work done against the wall adhesion force is always positive as it necessarily opposes the displacement.

The second law of thermodynamics requires that in any natural process $\delta\tilde{A}\leq 0$. Therefore, for equilibrium to be stable, $\tilde{A}$ must always have attained a minimum value. From equation (6), it follows that, provided the inequality:

$$F_{DF}+F_B\leq\left|F_w\right| \qquad (7)$$

is satisfied, both positive or negative values of the displacement δx result in an increase in $\tilde{A}$, implying that $\tilde{A}$ is at a minimum and hence that stable equilibrium can always be achieved. However, if the inequality is not satisfied, a positive displacement δx always results in a reduction in $\tilde{A}$, implying that stable equilibrium is no longer possible and the bubble must slide along the surface indefinitely in the x direction. Inequality (7) thus provides the condition for stability of the bubble against sliding. The forces appearing in the inequality are evaluated below.

2.3.1 Wall adhesion force (F_w)

The origin of the wall adhesion force is the well-known phenomenon of hysteresis of the value of the thermodynamic contact angle θ^* observed in wetting (when the liquid front is advancing) and de-wetting (when the liquid front is receding) processes. As reported in many texts (see for example Ref. [19]), for fluid/surface combinations of practical interest, at the point of breakdown of equilibrium, the contact angle for wetting (i.e. the 'advancing' contact angle, θ_a^*) is observed to be greater than that for de-wetting (i.e. the 'receding' contact angle, θ_r^*). Klausner et al. [5] assumed that for the case of an attached bubble in a flowing liquid at the point of sliding, the contact angle at the downstream edge of the contact line would be θ_r^* and that at the upstream edge would be θ_a^*. They derived a value for the net adhesion force opposing sliding by integrating the surface tension force along the contact line, assuming a particular variation in the contact angle between these locations.

An alternative to the Ref. [5] method for finding F_w that does not involve making assumptions about the variation of the contact angle along the contact line, is to adopt an energy-based approach in which the Young-Laplace equation is used to relate the equilibrium contact angle to the surface energies of the vapour-liquid, solid-vapour and solid-liquid interfaces [20]. The Young-Laplace equation states that, in the absence of external forces, the equilibrium contact angle is given by:

$$cos\,\theta^* = \frac{\left(\sigma_g - \sigma_f\right)}{\sigma} = \frac{\Delta\sigma}{\sigma} \quad (8).$$

Applying the reasoning used to derive the Young-Laplace equation to the case of an advancing or receding liquid front at the point of the breakdown of equilibrium, leads to the equivalent equations:

$$\begin{aligned} cos\,\theta_a^* &= \frac{\Delta\sigma_a}{\sigma} \\ cos\,\theta_r^* &= \frac{\Delta\sigma_r}{\sigma} \end{aligned} \quad (9)$$

where $\Delta\sigma_a$ and $\Delta\sigma_r$ are the differences between the specific surface energies of the solid-vapour and solid-liquid interfaces during wetting and de-wetting of the surface, respectively. From an energy point of view, $\Delta\sigma_a$ can be identified as the energy required to wet a unit area of the dry surface, and $\Delta\sigma_r$ with the energy that is released in de-wetting unit area of a wetted surface.

When an attached bubble is displaced by amount δx, a portion of the surface is wetted and another portion de-wetted. It is shown in the Appendix that the net work done is equal to

$$F_w\left|\delta x\right| = D_b\left|\delta x\right|\left(\Delta\sigma_r - \Delta\sigma_a\right) \quad (10),$$

where D_b is the diameter of the bubble base. Equation (10) expresses the wall adhesion force, F_w, in terms of the known diameter of the bubble base and $\Delta\sigma_a$ and $\Delta\sigma_r$, which are properties of the fluid and the surface.

To find $\Delta\sigma_a$ and $\Delta\sigma_r$ for an unknown surface we assume that the contact angle deviates from the average thermodynamic equilibrium value θ^* by an as yet unknown factor ε that is a property of the fluid/surface system:

$$\begin{aligned} \theta_r^* &\equiv \left(1-\varepsilon\right)\theta^* \\ \theta_a^* &\equiv \left(1+\varepsilon\right)\theta^* \end{aligned} \quad (11).$$

The factor ε is assumed much smaller than unity, which allows truncating the cosine series expansion after the second order term. Then equations (10) and (11) can be used to approximate $F_w|\delta x|$ in terms of the bubble base diameter D_b, the mean equilibrium contact angle θ^* and the factor ε, as

$$F_w\left|\delta x\right| \simeq 2\varepsilon\left|\delta x\right| D_b\sigma\theta^* \quad (12),$$

where θ^* is in radians.

2.3.2 Drag force (F_{FD})

Given the typically small (less than one millimeter) bubble diameters and the typical values of the imposed liquid velocity (around or less than one metre per second), the drag force in the direction of the imposed flow is expected to be primarily due to molecular viscosity. Following Ref. [21] the drag force is therefore computed from the Stokes law for a rigid sphere [22], modified by a correction factor C_{FD} accounting for possible deviations from the viscous flow solution at higher liquid mass flow rates. This leads to the following equations for the drag force:

$$\begin{aligned} F_{FD} &= 6C_{FD}\pi\rho_f\nu R_{EQ}\Delta U \\ C_{FD} &= \frac{2}{3}+\left[\left(\frac{12}{Re_B}\right)^{0.65}+0.796^{0.65}\right]^{-1.54} \end{aligned} \quad (13),$$

In equation (13), ν is the kinematic viscosity of the liquid, R_{EQ} is the equivalent radius of a spherical bubble of the same volume of the actual bubble, and the velocity difference ΔU between the stationary bubble and the liquid is evaluated at the elevation of the bubble centroid.

2.3.3 Buoyancy force (F_{Bx})

F_{Bx} is the component of the buoyancy force in the direction parallel to the surface:

$$F_{Bx} = \frac{4}{3}\pi R^3 \phi_1 \rho_f g \sin\gamma \quad (14).$$

2.3.4 Final form of the condition for equilibrium against sliding

With the definitions above, the final form of the equation expressing the condition of equilibrium against sliding is, in non-dimensional form:

$$6C_{FD}\pi\phi_1^{1/3}\nu^+U^+ + \frac{4}{3}\pi\phi_1 R^{+2}\sin\gamma - 4\varepsilon\theta^*\sin\theta = 0 \quad (15),$$

where the non-dimensional kinematic viscosity of the liquid is defined as $\nu^+ = \nu\left(\frac{\rho_f^3 g}{\sigma^3}\right)^{1/4}$.

2.4 <u>Solution approach</u>

Solution of equation (5) for θ requires knowledge of the bubble radius R^+ and, in principle, also of the growth rate $\dot{R}^+$ at each time step, with the terms in $\dot{R}^+$ representing the work done against fluid reaction forces associated with bubble expansion. In practice bubble growth rates depend on the Jakob number $Ja = \frac{c_f\rho_f\Delta T_w}{\rho_g h_{fg}}$, where c_f is the liquid specific heat capacity, ΔT_w is the wall superheat, and h_{fg} is the latent heat of vaporization. It was found in Ref. [11] that at Jakob numbers smaller than ~20, the influence of fluid reaction forces on θ is insignificant, and that the former only become really important at Jakob numbers above ~100. Flow boiling is characterized by high heat transfer rate and moderate wall superheats, typically corresponding to Jakob numbers well below 20, and usually less than 5. At high pressures, the reduced density ratios ρ_f/ρ_g result in even smaller Jakob numbers, typically <1.

It is thus possible to neglect terms in $\dot{R}^+$ in equation (5) that represent the reaction forces due to the bubble expanding into the surrounding body of liquid. This simplifies the analysis considerably, as it makes the computation of bubble growth rates unnecessary for computing the bubble departure diameter. This simplification constitutes a significant difference between the present model and previous models reported in refs. [6], [5, 16], [9], which required an estimate to be made of the bubble growth rate; the latter was usually obtained from experimental observations or other kinds of fits, but never computed mechanistically.

To find the bubble departure diameter using the current model, equation (5) is solved numerically for θ for increasing[1] values of the bubble radius R^+. At each step, equation (15) is applied to check that the bubble is stable against sliding. The bubble departure

[1] Sensitivity of the solution procedure to the small increments in R+ has been checked via a convergence study. Values of the increment below 0.001 were found to return increment-independent solutions.

diameter is taken as the smallest diameter that satisfies either the condition $\theta = 0$, or at which equation (15) is satisfied. The first case represents bubble detachment via lift-off, the second represents bubble departure via sliding.

The only unknown quantity appearing in the model is the parameter ε, which describes the hysteresis between the advancing and receding contact angles at the point of the breakdown of equilibrium. A value of ε to be used with the model is suggested in Section 3 by optimizing the fit to test data.

3 OPTIMIZATION OF THE CONTACT ANGLE HYSTERESIS PARAMETER

In order to establish an optimum value for the (unknown) parameter ε, used to account for contact angle hysteresis, a parametric study was conducted in which predictions of the departure diameter made using equations (5) and (15) for different values of ε were compared against measurements from several data sources, as summarized in Table 1.

	Ref. [5, 16]	Ref. [18]	Ref. [23]	Ref. [24]	Ref. [25]
Fluid	Refrigerant r113	Refrigerant FC-87	Water	Water	Water
Boiling regime	Horizontal stratified flow (saturated)	Subcooled	Subcooled	Subcooled	Subcooled
Inclination angle γ [°]	0	90, upflow and downflow	0-90-120-135-150-180	90	90
Pressure [bar]	1	1	1-5	1	1-3
Mass flux $[kg/m^2/s]$	113-315	192-319	250-400	466-900	76.6-766
Subcooling [°C]	0	2-5	10,20	2-20	10,20,30

Table 1
Summary of experimental data used for determining contact angle hysteresis parameter.

For each experimental point, the absolute value of the discrepancy between predicted and measured departure diameter was evaluated for three different values of the parameter ε, equal to 0.035, 0.07 and 0.14. Assuming a value of θ^* of 40°, typical of low-pressure boiling, the values of ε correspond to values of the advancing and receding contact angles of, respectively, $(40.0 \pm 1.4)°$, $(40.0 \pm 2.8)°$and $(40.0 \pm 5.6)°$. Yeoh et al. [8] conducted a survey of contact angle measurements in low pressure boiling for various fluid/surface combinations and found similar values, finally adopting $(40.0 \pm 5.0)°$ for the advancing/receding contact angles for his own modelling work. Hence the assumed range of values for ε is consistent with previous estimates.

From the cumulative error distributions obtained via the parametric study, shown in Figure 2, values of the Mean Absolute Error (MAE) and Root Mean Square (RMS) error of predictions of the current model have been extracted.

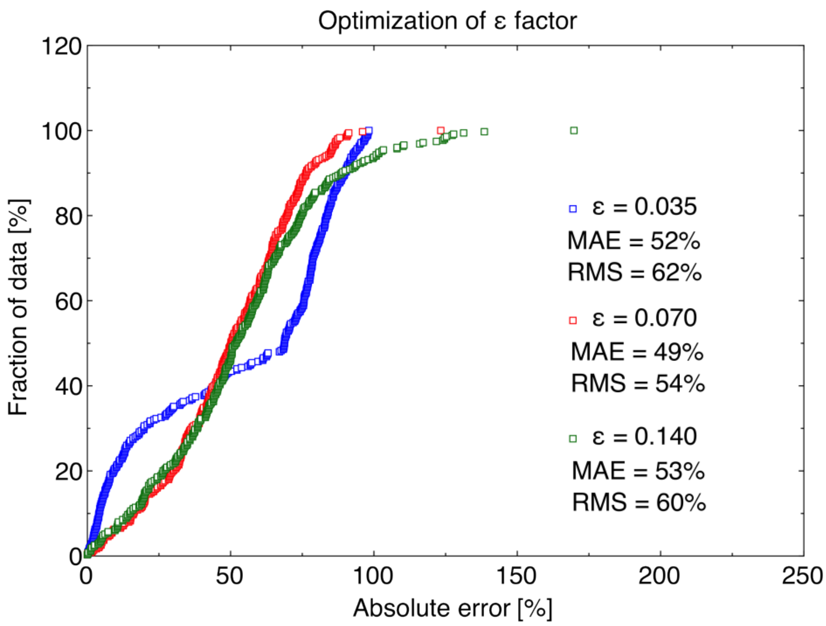

Figure 2
Distribution of the errors of predictions obtained with the current model for three values of the contact angle hysteresis parameter ε.

As shown in Figure 3, the parametric study suggests that using a choice of ε value of 0.07 minimizes the overall error in predictions of departure diameters. The value was therefore used in subsequent applications of the model.

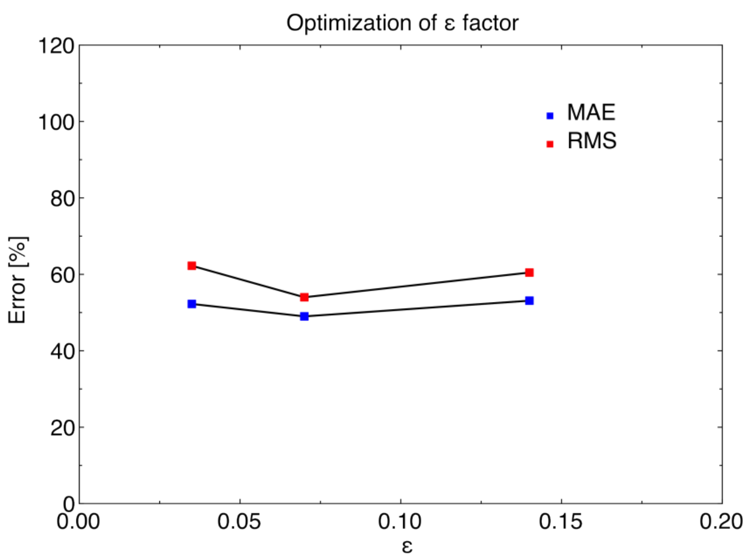

Figure 3
Variation of the average errors of predicted bubble departure diameters as a function of

the contact angle hysteresis parameter, evaluated used the databases summarized in Table 1.

4 ASSESSMENT OF THE MODEL PREDICTIONS OF EXPERIMENTAL TRENDS

4.1 The experiments of ref. [23]

Sugrue et al. [23] conducted a comprehensive program of experiments to investigate the influence of subcooling, flow velocity and orientation of the boiling surface on bubble departure diameters in flow boiling of water in a square channel, at pressure up to 5 bars. The data are particularly useful in allowing the predicted effect on departure diameter of pressure, liquid flow velocity and surface inclination to be *separately* tested.

The data were used to test the ability of the current model to describe the observed variation of bubble departure diameter with pressure, liquid flow velocity and surface inclination.

4.1.1 Modelled and measured bubble departure diameters

The predicted effect of increasing system pressure on departure diameter is compared with test data in Figure 4. The departure diameter is observed to fall with increasing system pressure and this trend is correctly predicted, as shown.

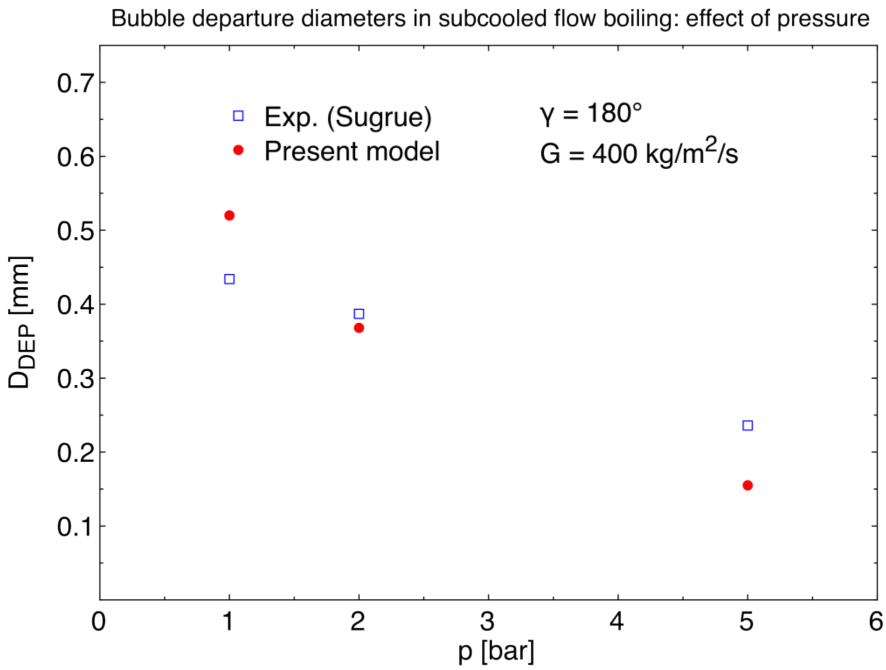

Figure 4
Effect of fluid pressure on bubble departure diameter at a downward-facing horizontal surface, subcooling of 10K and heat flux of 50,000 W/m^2. Showing comparison with the experiments of ref. [23].

The predicted effect of the surface inclination γ on the bubble departure diameter is compared with measurements in Figure 5. Model predictions are in reasonable agreement with the measured data, although an offset between modeled and measured bubble departure diameters is observed.

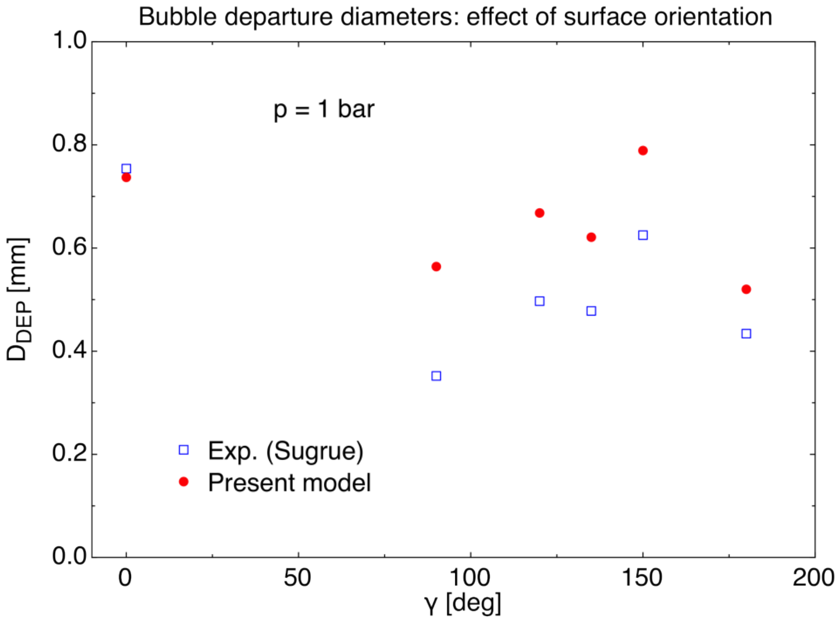

Figure 5
Variation of bubble departure diameters with surface orientation, at a mass flux of 250 kg/m^2/s, subcooling of 10K and heat flux of 50,000 W/m^2. Showing comparison between the present model and experimental data from the database of ref. [23].

The rather weak effect of inclination seen in both the measured data and model predictions in Figure 5 indicate that for the particular experimental conditions, the drag force and lift forces due to the imposed flow (which do not depend on the orientation angle) are dominant over gravitational forces.

To investigate the effect of flow velocity on bubble departure diameter, test results for a downward-facing horizontal surface ($\gamma = 180°$) were analysed. For a downward facing surface, the only possible mechanism of departure is that via sliding due to the action of drag and lift forces. Experimental results are plotted as hollow symbols against mass velocity for three different pressures in Figure 6. As expected the departure diameters decrease with increasing mass velocity. The current model, whose predictions are plotted as full symbols, reproduces the observed trends reliably, although the effect of pressure on departure diameter is somewhat overestimated.

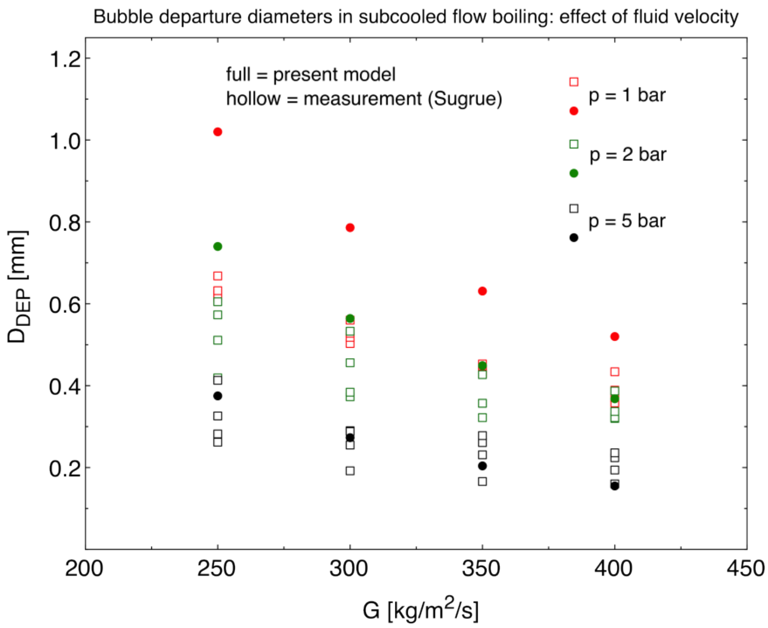

Figure 6
Effect of flow velocity on bubble departure diameter. Showing variation of the bubble departure diameter with the mass flux of liquid, at different pressures, for the case of bubble growth at a downward facing horizontal surface ($\gamma = 180°$). For each value of pressure and mass flux, experimental points are shown at heat fluxes are of 50,000 W/m^2 and 100,000 W/m^2 and subcooling values of 10K and 20K.

In conclusion to this section, it is helpful to reiterate that the separate effects of pressure and inclination angle on bubble departure diameters are captured by the current model, as opposed to the previous Klausner and Yun models, which where shown in Ref. [23] to return rather poor predictions in the same conditions.

5 COMPARISON WITH EXISTING BUBBLE DEPARTURE MODELS

Sugrue et al. [9, 23] provided a statistical survey on the performance of existing models for predicting bubble departure diameter in flow boiling against a large database of experimental results, including the tests analysed in Section 4, above, as well as those of Situ et al. [24] and Prodanovic et al. [25], involving subcooled boiling of water in vertical upflow. The complete database corresponds to the tests identified in Table 1 in Section 3. Predictions of the current model were compared with experimental results in the same database and compared with predictions of existing models.

Figure 7 and Figure 8 compare the database results with predictions of the current model, and three existing models based on the force-balance approach. Results are plotted in terms of the statistical distribution of the absolute error in the predictions: the overall error is quantified in terms of mean absolute error (MAE), and the root mean square error (RMS). As shown in the figures, the MAE and RMS errors obtained with the present model are smaller than those obtained with the Klausner model [5], and comparable with those obtained with the Yun model [6]. Errors are slightly larger than those obtained with optimised fit to data proposed by Sugrue in Ref. [9]. However the earlier models relied to some degree on empirical fitting, using experimentally observed data, notably for the advancing and receding contact angles, the surface area of the bubble base that is in contact with the solid surface, and the bubble growth rate. Beyond the use of the parameter ε describing the hysteresis between the advancing and receding contact angles, which is deduced from data fitting, the present model is purely predictive, requiring no information on other experimental parameters. The avoidance of fitting parameters gives confidence in the ability of the current model to describe bubble departure in conditions that are outside the range of the database, notably boiling at high pressures encountered in many industrial applications.

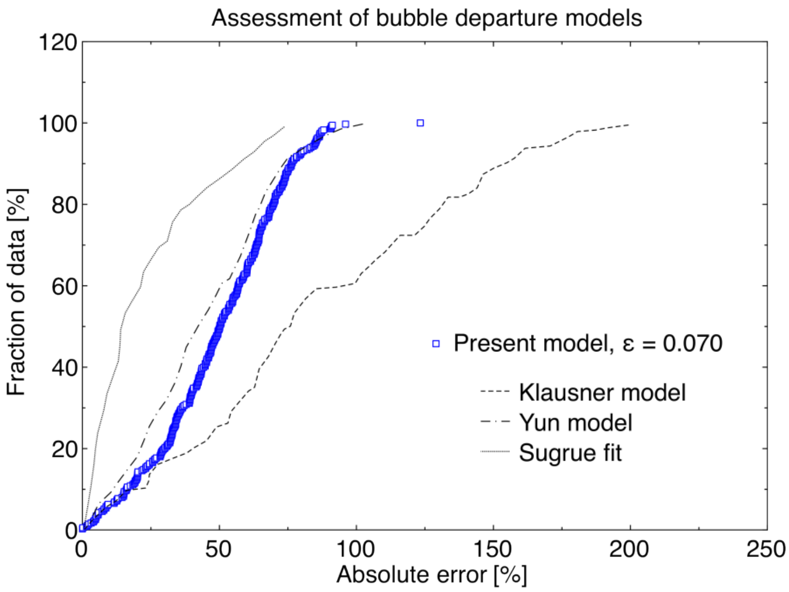

Figure 7
Assessment of bubble departure models using the datasets summarized in Table 1.

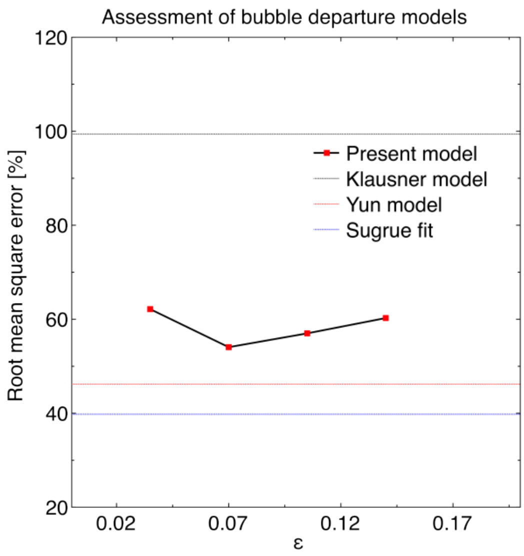

Figure 8
Assessment of the performance of the current bubble departure model versus the performance of extant models. Root mean square errors of the present model are shown for different values of the contact angle hysteresis parameter ε. A value of ε of 0.07 is seen to minimize the error of the present model.

6 DISCUSSION AND CONCLUSIONS

A method for predicting bubble departure diameters in flow boiling has been developed based on the principle that the free energy of an attached bubble in equilibrium must always be at a minimum. The model has been compared with departure diameters in existing experimental databases and has been shown to give agreement that is comparable or superior to that obtained with previous models, which have generally used a force-balance approach. The new model offers a number of advantages over the previous methods as follows:

- The contact area between the bubble and the heated surface (which is crucially important for determining the surface tension forces acting on the bubble) is an output of the current energy-based model. In the force-balance approach, the contact area is generally treated as an input parameter as no means are available for establishing its magnitude. The availability of a physically based predictive method for contact area increases the confidence in the applicability of the current energy-based approach when applied outside the range of current data (e.g. to high pressure boiling).
- In contrast to the force-based methods, the current energy-based model shows that, in typical flow boiling conditions, fluid reaction forces acting on the bubble due to its radial expansion can be neglected in comparison with the surface tension forces. Previous force-balance models (see for example Ref. [15]) have considered that fluid reaction force due to bubble growth to be dominant over

surface tension forces, and therefore require the bubble growth rate to be calculated as part of the calculation of the departure diameter. The present work suggests that previous understanding of the magnitude of relevant forces is erroneous, and fluid reaction forces due to the bubble's radial growth can in practice be neglected in bubble departure in flow boiling: this allows bubble departure sizes to be obtained by a simple iterative solution of two implicit equations [(5) and (15)], greatly simplifying the departure diameter calculation compared with the force-balance approach.

- The only unknown parameters appearing in the current model are the thermodynamic equilibrium contact angle θ^* and the dimensionless parameter ε used to relate the advancing and receding contact angles to θ^*. Estimates of θ^* and ε have been proposed which, used with the current model, result in a good fit to measured bubble departure diameter in both forced convection boiling and pool boiling for a wide range of pressures and different fluids. Models for bubble departure size using the force-balance method have generally required numerous additional parameters to be specified. The reduced reliance on adjustable parameters in the current model gives increased confidence in its applicability to describe bubble departure for conditions where data is limited such as boiling at high pressures.

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8 APPENDIX – DERIVATION OF EQUATION (10)

We consider a small displacement of the bubble base, whose area SF is assumed to remain unchanged. For *any arbitrary shape* of the bubble base, the net change in surface energy due to the displacement can be computed, as shown in the schematic of Figure 9 (depicting the case, relevant here, of a circular bubble base), from the displacement δx and the perpendicular height D_b of the base area in the direction normal to δx. Considering the areas indicated in the figure, SB remains dry, SA is dewetted, SC is wetted, and the area SE is first dewetted and then rewetted. Changes in specific free energy are, thus, respectively, $\Delta\sigma_r$ for area SA, $-\Delta\sigma_a$ for area SC, $\Delta\sigma_r - \Delta\sigma_a$ for area SE, and zero for area SB. The area of each of the circles is SF.

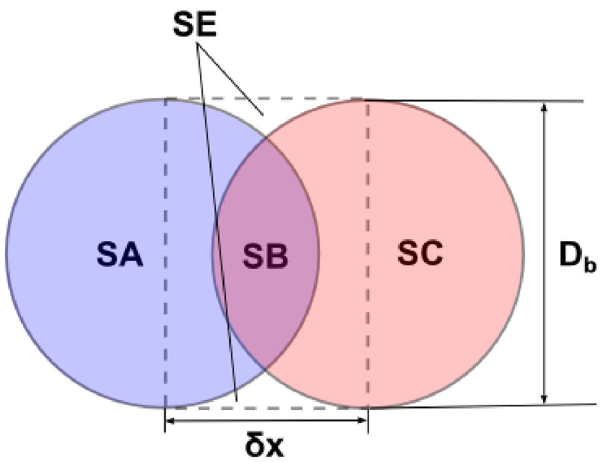

Figure 9
Sketch of the circular bubble base, used to compute the wall-adhesion term of equation (10), expressing equilibrium of the bubble against sliding.

The work done by wall adhesion forces can be computed as

$$\begin{aligned}&-\left(SF-SB\right)\Delta\sigma_a+\left(SF-SB\right)\Delta\sigma_r+\\&+\left[D_b\delta x-\left(SF-SB\right)\right]\left(\Delta\sigma_r-\Delta\sigma_a\right)=D_b\delta x\left(\Delta\sigma_r-\Delta\sigma_a\right)\end{aligned} \quad (16).$$

Equation (16) is equation (10) of the main body of text.

Conflict of interest

None declared.