A mechanistic model of vapour bubble departure in forced convection boiling

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1 Introduction

Nucleate boiling and two-phase flow behaviour have been studied for decades. Nevertheless, these are still thriving research areas within engineering, and thermal hydraulics in particular. The ability to predict two-phase boiling flow behaviour is of significant interest for the safe operation of boiling water reactors (BWRs), and in the design of new passive nuclear reactor systems operating on natural circulation. The development of computational fluid dynamic (CFD) approaches for predicting such flows has proved promising and of use in engineering design, in particular with the use of Eulerian averaged models. In this kind of model the phases are treated as interpenetrating continua with all the information on the interface structure lost due to the averaging process. Consequently, models are needed for the interphase exchanges of mass, momentum and energy to close the system of equations. In particular, a specific model is needed to describe nucleate boiling at the wall. Heat flux partitioning models, such as that of Kurul and Podowski (1990), have been adopted in most CFD models of boiling flows to date. This evaluates the amount of vapour generated from several parameters, such as the active nucleation site density, the bubble departure diameter and the bubble departure frequency.

Normally, in commercial CFD codes the bubble departure diameter is evaluated from empirical correlations, such as those by Tolubinsky and Kostanchuk (1970) and Kocamustafaogullari (1983). These simple correlations are limited to the effect of sub-cooling and/or system pressure.

More recently, mechanistic models have been developed to account for all the complex phenomena involved. Klausner et al. (1993) proposed a model based on a balance of the forces acting on the bubble during its growth phase and leading to bubble departure. Zeng et al. (1993) extended the original model to both pool and flow boiling conditions. Over the years, slightly modified versions of the Klausner et al. (1993) model have been used by many authors to predict their own experimental data (e.g. Situ et al., 2005; Wu et al., 2008; Yun et al., 2012). The introduction of different improvements based on validation against specific databases resulted in a large number of relatively accurate, but not extensively validated, models. In a more recent work, Sugrue and Buongiorno (2013) proposed a modified version of this model, showing improved accuracy with respect to both Klausner et al. (1993) and Yun et al. (2012). In their work, Sugrue and Buongiorno (2013) provide an extensive validation of the model against numerous datasets, showing in general good agreement. However, higher errors are observed against the database of Situ et al. (2005), which measured the diameter of bubbles at lift-off from the wall.

In all these models, a lot of attention is placed on the evaluation of the bubble growth phase. In the majority of cases, bubble growth is sustained by heat coming from the superheated layer around the bubble surface. Extended use is made of the models from Plesset and Zwick (1954), Zuber (1961) and Mikic et al. (1970). Accordingly to recent experimental observations (Gerardi et al., 2010), evaporation of the liquid microlayer under the bubble is identified as the leading mechanism sustaining the growth of the bubble. Models of bubble growth based on microlayer evaporation have been proposed by Copper and Loyd (1969) and Unal (1976). Nevertheless, there is no general agreement on the relative weight of the different mechanisms, as other experiments suggests a more limited effect of microlayer evaporation with respect to evaporation from the superheated liquid around bubble surface (Kim, 2009).

A significant number of experimental works on bubble growth and bubble departure diameter have been published and are available for model validation. Among others, relevant works are due to Unal (1976), Bibeau and Salcudean (1994), Throncroft et al. (1998), Prodanovic et al. (2002), Situ et al. (2005), Chen et al. (2009) and Sugrue (2012). More recently, the evolution of experimental techniques allowed very detailed measurements of the bubble growth phase, including wall temperature distribution and dry area under the bubble (Demiray and Kim, 2004; Gerardi et al., 2010).

In this paper, starting from the mechanistic model of Klausner et al. (1993), modifications are introduced in some of the terms of the force balance. Between the different forces, surface tension, drag force, shear lift force, buoyancy and liquid displacement due to bubble growth are identified as the dominant ones. Some modifications are introduced in the surface tension force parameters and a new equation governing bubble growth is proposed. The new formulation accounts for evaporation of the microlayer under the bubble and heat transfer from superheated and sub-cooled liquid around the bubble surface. To the authors' knowledge, no attempt has yet been made to include all the possible heat transfer contributions in a mechanistic model for bubble departure diameter. A pioneering model for bubble growth due to Van Stralen et al. (1975) included microlayer evaporation and heat transfer from the superheated liquid. Recently, Yun et al. (2012) included condensation around the bubble coupled with heat transfer from the superheated liquid. The model developed is compared to three datasets for sub-cooled flow boiling of water (Prodanovic et al. (2002), Situ et al. (2005) and Sugrue (2012)) and the data of Klausner et al. (1993) for saturated flow boiling of refrigerant R113. The whole database allows validation of the model over a broad range of experimental parameters and operating conditions. In addition, the model's ability to predict bubble lift-off other than bubble departure diameter is evaluated using the data of Situ et al. (2005). Experimental data and the new mechanistic model are presented in Sections 2 and 3. Section 4 contains preliminary validation of the bubble growth equation, with global comparisons with experiments provided in Section 5. Conclusions and future developments are drawn in Section 6.

2 Experimental databases

In this paper, three databases of sub-cooled flow boiling of water are used for model validation, i.e. those of Prodanovic et al. (2002), Situ et al. (2005) and Sugrue (2012). These combined databases allow an extensive validation over wide ranges of mass flux, heat flux and inlet sub-cooling (250 kg m^{-2} s^{-1} < G < 900 kg m^{-2} s^{-1}, 50 kW m^{-2} < q'' < 1200 kW m^{-2}, 1.5 °C < ΔT_{sub} < 60 °C). The system pressure is considered to be in the range 1-5 bar. An additional comparison is made with data from Klausner et al. (1993), related to the saturated boiling of refrigerant R113. The details of each database are summarised in Table 1.

A first comparison has been made between the experimental data and correlations of Tolubinsky and Kostanchuk (1970) and Kocamustafaogullari (1983). Both are normally implemented in commercial CFD codes for calculation of the bubble departure diameter. In Figure 1 they are compared with the data of Sugrue (2012), whilst in **Error! Reference source not found.** the data of Klausner et al. (1993) are compared with the correlation of Kocamustafaogullari (1983). As shown in the figures, large discrepancies are found between predictions from these correlations and the experimental data. Significant physical effects, which are clearly evident from the experiments, such as mass flow rate and thermal flux, are neglected in their formulations. Therefore, these results suggest the need for an improved and more detailed mechanistic model for bubble departure in the context of the CFD simulation of boiling flows.

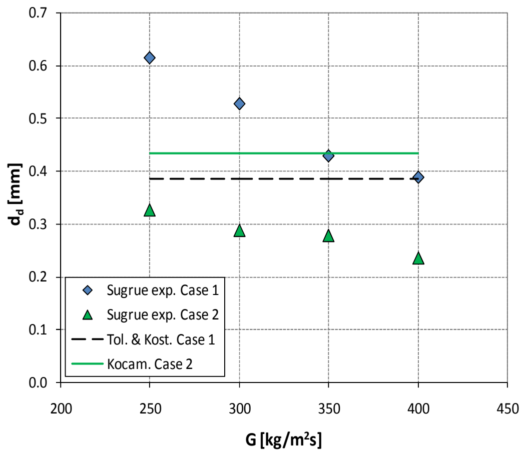

Figure 1: Comparison between the experimental data of Sugrue (2012) and the correlations of Tolubinsky and Kostanchuk (1970) and Kocamustafaogullari (1983). Case 1: p = 1.01 bar, ΔT_{sub} = 20 °C, q'' = 50 kW m^{-2}; Case 2: p = 5.05 bar, ΔT_{sub} = 10 °C, q'' = 100 kW m^{-2}.

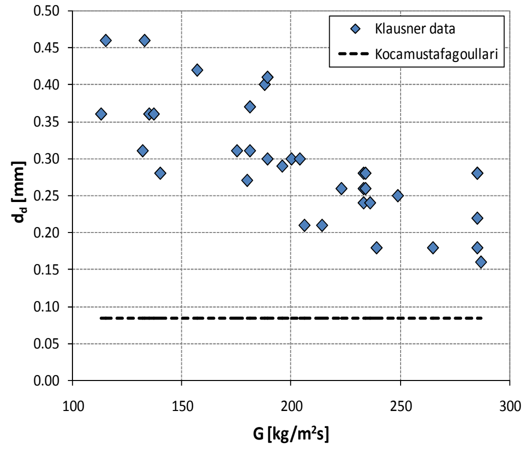

Figure 2: Comparison between the experimental data of Klausner et al. (1993) and the correlation of Kocamustafaogullari (1983).

3 Mechanistic model

The model developed by Klausner et al. (1993) is based on a force balance acting on a single nucleation site. The balance of forces is carried out in both directions, parallel (x-direction) and perpendicular (y-direction) to the flow direction:

$$\sum F_x = F_{stx} + F_{qsd} + F_b \sin\theta + F_{udx} = 0 \quad (1)$$

Table 1. Databases used for validation of the bubble departure diameter model.

	Sugrue (2012)	Situ et al. (2005)	Prodanovic et al. (2002)	Klausner et al. (1993)
Fluid	Water	Water	Water	R113
Orientation	0°,30°,45°,60°,90°,180°	Vertical	Vertical	Horizontal
Channel	Rect.; D_h =16.7 mm	Ann.; D_h=19.1 mm	Ann.; D_h=9.3 mm	Rect.; D_h=25 mm
G / kgm^{-2}s^{-1}	250 - 400	466 - 900	76.6 - 766	112 - 287
q″ / kWm^{-2}	50, 100	54 - 206	200 - 1000	11 - 26
ΔT_{sub} / °C	10, 20	2 - 20	10, 20, 30	Saturated
p / bar	1.01, 2.02, 5.05	1.01	1.05 - 3.00	1.01

$$\sum F_y = F_{sty} + F_{sl} + F_b \cos\theta + F_{udy} = 0 \quad (2)$$

In the previous equations, F_{st} is the surface tension force, F_{qsd} is the quasi- steady drag force, F_b is the buoyancy force, F_{sl} is the shear lift force and F_{ud} is the unsteady drag force due to bubble growth. Whilst the sum of the forces in both directions equals zero, the bubble grows from the nucleation site without detaching. Detachment occurs when Eq. (1) or Eq. (2) is violated and detaching forces overcome forces that prevent bubble departure. If the x-direction balance is violated before the y-direction balance, the bubble departs from the nucleation site and slides along the heated wall. Conversely, the bubble lifts-off from the wall without sliding. For quasi-steady drag, shear lift and unsteady drag, the same models from Klausner et al. (1993) are used. The surface tension force in the x-direction is expressed as:

$$F_{stx} = -1.25 d_w \sigma \frac{\pi(\alpha-\beta)}{\pi^2-(\alpha-\beta)^2}(\sin\alpha - \sin\beta) \quad (3)$$

and in the y-direction:

$$F_{sty} = -d_w \sigma \frac{\pi}{(\alpha-\beta)}(\cos\beta - \cos\alpha) \quad (4)$$

In the previous equations, α is the advancing contact angle, β the receding contact angle and d_w the contact diameter between the bubble and the heated surface. Measurements and reliable models for these parameters are rather scarce in the literature, therefore they are one of the major sources of uncertainty in the present model. Klausner et al. (1993) recommended $\alpha = \pi/4$ and $\beta = \pi/5$ from their measurements in R113. For the contact diameter d_w, a value of 0.09 mm was given. Instead, a constant ratio with bubble diameter $d_w = d_B/15$ was used by Yun et al. (2012). Some measurements of contact angles have been provided by Sugrue (2012) for water, namely 90.63° for the advancing and 8.03° for the receding contact angle. In addition, a much lower contact diameter to bubble diameter constant ratio was reported to give fairly good agreement with data. In this work, the suggestions from Klausner et al. (1993) for contact angles and the Yun et al. (2012) formulation for contact diameter are generally used. By virtue of the good agreement reported, values from Sugrue (2012) are employed to predict the latter database.

Prior to departure, bubble diameter behaviour is governed by a growth equation. During growth, bubbles are assumed hemispherical in the present model. Moreover, only the asymptotic phase of the bubble growth is considered, which is characterised by the diffusion of heat from the surrounding liquid. Conversely, inertia controlled bubble growth has been neglected. This hypothesis is justified by the very short duration of this growth phase (Unal, 1976). Differently from the majority of other available models, the present formulation includes the evaporation of the thin liquid microlayer formed under the bubble during its growth. As reported, this microlayer can be considered as the dominant, or at least a significant, energy source during bubble growth (Gerardi et al., 2010). Microlayer evaporation is evaluated accordingly to the model proposed by Cooper and Lloyd (1969):

$$\frac{dR(t)}{dt} = \frac{2}{C_2} Pr^{-0.5} Ja \left(\frac{k_l}{\rho_l C_{p,l}}\right)^{0.5} t^{-0.5} \tag{5}$$

The constant C_2 is related to the initial width of the microlayer. After optimisation with the experimental databases, a value of 1.78 is used in this work, higher than the value estimated by Copper and Lloyd (1969) between 0.8 and 1.2. A higher value is to be expected since the value from Copper and Lloyd (1969) was calculated considering only the microlayer contribution to bubble growth. Instead, the present model accounts also for the heat provided by the superheated boundary layer across the bubble surface. In his review paper, Kim (2009) states that the major contribution to bubble growth comes from heat diffusion from the superheated boundary layer. Therefore, it seems reasonable to account for both contributions to develop a general bubble growth model applicable in all conditions. The superheating contribution is based on the model developed by Plesset and Zwick (1954):

$$\frac{dR(t)}{dt} = \sqrt{\frac{3}{\pi}} k_l (T_l - T_{sat}) \left(\frac{k_l}{\rho_l C_{p,l}}\right)^{0.5} t^{-0.5} \tag{6}$$

Finally, condensation on the bubble cap as it comes in contact with the sub-cooled liquid is accounted for. The condensation heat transfer coefficient is evaluated from the Ranz and Marshall (1952) correlation:

$$h_c = \frac{k_l}{d_B}(2 + 0.6 Re^{0.5} Pr^{0.3}) \tag{7}$$

The complete bubble growth equation then reads:

$$\frac{dR(t)}{dt} = \frac{2}{C_2} Pr^{-0.5} Ja \left(\frac{k_l}{\rho_l C_{p,l}}\right)^{0.5} t^{-0.5} + \sqrt{\frac{3}{\pi}} k_l (T - T_{sat}) \left(\frac{k_l}{\rho_l C_{p,l}}\right)^{0.5} (1-b) t^{-0.5} + - \frac{h_c}{\rho_v h_{lv}} (T_{sat} - T_{sub}) b \tag{8}$$

The parameter *b* determines the portion of the bubble surface in contact with the sub-cooled liquid. It is calculated determining the location of the saturation temperature in the boundary layer from a temperature profile scaled on the single-phase wall function from Kader (1981):

$$\theta^+ = Pr y^+ e^{-\Gamma} + \left\{ 2.12 \ln \left[(1 + y^+) \frac{2.5\left(2 - {}^{y}/_{\delta}\right)}{1 + 4(y - \delta)^2} \right] + \beta(Pr) \right\} e^{-1/\Gamma} \tag{9}$$

where:

$$\beta(Pr) = \left(3.85 Pr^{1/3} - 1.3\right)^2 + 2.12 \ln Pr \tag{10}$$

and:

$$\Gamma = \frac{0.01 (Pr y^+)^4}{1 + 5 Pr^3 y^+} \tag{11}$$

Since the wall temperature is not provided for all the experiments considered, it is calculated from the correlation of Chen (1966). This correlation assumes the total heat transfer coefficient as the superposition of a convective contribution and a nucleate boiling contribution:

$$h_{tp} = h_{conv} + h_{nb} \tag{12}$$

The convective component is represented as a Dittus-Boelter type equation:

$$h_{conv} = 0.023 \left[\frac{G(1-x)D_h}{\mu_l}\right]^{0.8} \left(\frac{\mu_l C_{p,l}}{k_l}\right)^{0.4} \left(\frac{k_l}{D_h}\right) F \tag{13}$$

whilst the nucleate boiling component uses a slight modification of the analysis by Foster and Zuber (1955):

$$h_{nb} = 0.00122 \left[\frac{k_l^{0.79} C_{p,l}^{0.45} \rho_l^{0.49}}{\sigma^{0.5} \mu_l^{0.29} i_{lv}^{0.24} \rho_v^{0.24}}\right] \Delta T_{sat}^{0.24} \Delta p_{sat}^{0.75} S \tag{14}$$

Knowledge of the temperature distribution allows calculation of the value of *b* and the average temperatures for the superheated and sub-cooled regions.

4 Preliminary validation of the growth phase

First, an evaluation of the accuracy of the bubble growth equation was made. The growth process described by Eq. (8) was compared with experimental growth transients from Prodanovic et al. (2002). An issue was identified in the sub-cooling correlation. Using the bubble diameter in Eq. (7) results in a too high a sub-cooling value in the first part of the transient, when the bubble diameter is small. Therefore, the hydraulic diameter was used in the following simulations. Growing transients are compared with two experiments in Figure 3 and Figure *4*, with satisfactory agreement found. As well as the bubble diameter, the separate contributions of the microlayer, superheating and sub-cooling are shown. A major contribution is provided by the microlayer evaporation, in agreement with the findings of Gerardi et al. (2010). Major discrepancies are found after the maximum bubble diameter is reached in the experiments. In its present formulation, therefore, the model is not able to handle bubble shrinking due to condensation. However, bubble condensation at the wall after departure but prior to lift-off is expected only for some of the data of Prodanovic et al. (2002), which are characterised by high values of liquid sub-cooling. In both Figure 3 and Figure 4 the effect of sub-cooling is rather small. Even if the sub-cooling temperature is not low, they are characterised by a high heat flux.

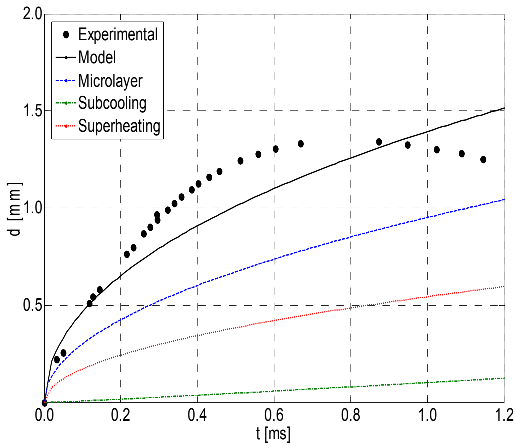

Figure 3: Comparison between the bubble growth model and a bubble growing transient from Prodanovic et al. (2002). p = 1.05 bar; G = 410.4 kg m^{-2}s^{-1}; q'' = 600 kW m^{-2}; ΔT_{sub} = 30°C.

For higher sub-cooling or lower heat fluxes, the contribution of sub-cooling becomes more relevant, as shown in Figure 5 for a set of conditions from Situ et al. (2005). In some limited situations, sub-cooling was observed to overcome the contribution from the superheated liquid layer around the bubble surface.

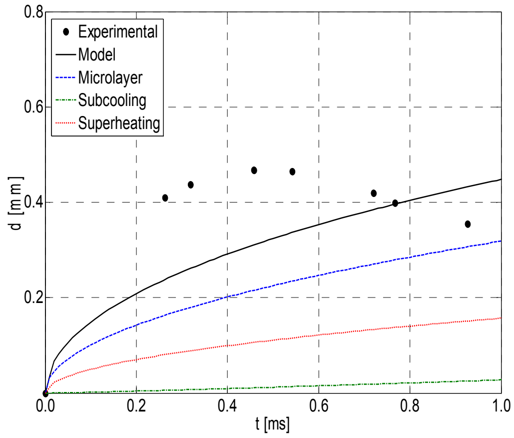

Figure 4: Comparison between the bubble growth model and a bubble growing transient from Prodanovic et al. (2002). p = 3 bar; G = 391.7 kg m^{-2}s^{-1}; q'' = 600 kW m^{-2}; ΔT_{sub} = 29.4°C.

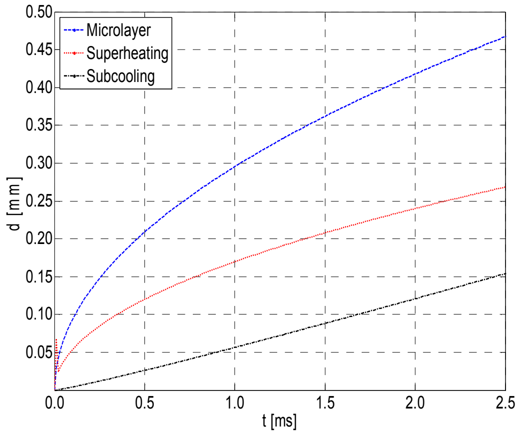

Figure 5: Simulated growing transient in experimental conditions of Situ et al. (2005). p =1 bar; G = 910.6 kg m^{-2}s^{-1}; q'' = 202 kW m^{-2}; ΔT_{sub} = 20°C.

5 Results and discussion

The complete model has been compared with the three databases of Prodanovic et al. (2002), Situ et al. (2005) and Sugrue (2012) for sub-cooled boiling at atmospheric pressure. The comparisons are shown in Figures 6, 7 and 8. The new model shows reasonable accuracy with a combined average relative error of 27.4% with respect to those data. Therefore, the ability to give accurate estimations over a broad range of conditions is demonstrated. Better accuracy is shown for the Sugrue (2012) and Situ et al. (2005) databases, with an average relative error of 19.0% and 24.3%, respectively. Higher errors are found for the database of Prodanovic et al. (2002), for which the average relative error is over 40%. The database of the latter authors seems the most difficult to predict, since comparable errors are found also in Sugrue and Buongiorno (2013).

It is important to focus the discussion on the comparison with Situ et al. (2005). Data for this database are related to bubble lift-off, whereas the other two include data for bubble departure. Predictions for bubble lift-off are obtained when the force balance in the y-direction is violated. When the balance in the x-direction is violated first, the calculation is carried on, neglecting the contact diameter between the bubble and the heated surface, and hence the surface tension force. The bubble lift-off diameter is then obtained when the balance in the y-direction is also violated. Therefore, the model seems able to predict not only the diameter of the bubble at departure, whether it slides on the heated surface or directly lifts-off from the surface, but also to some extent the lift-off diameter after bubble sliding.

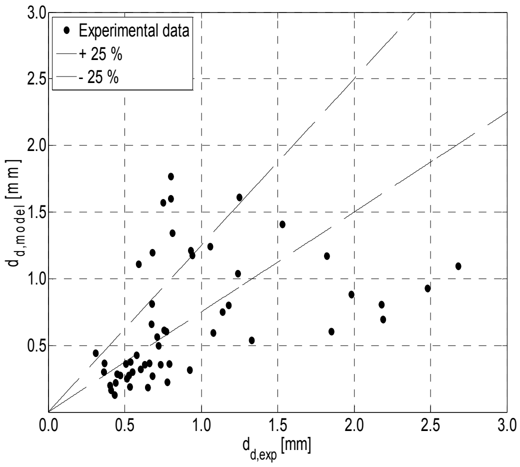

Figure 6: Comparison between model predictions and experimental data of Prodanovic et al. (2002).

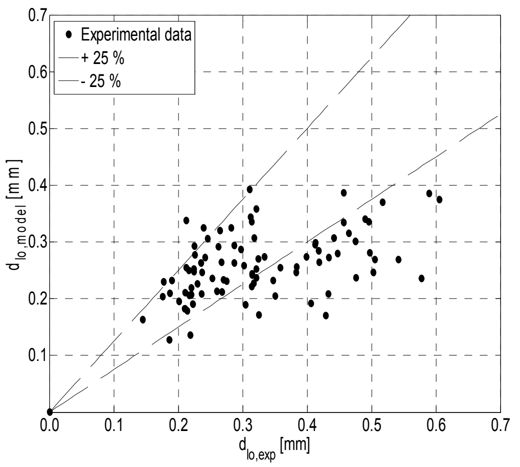

Figure 7: Comparison between model predictions and experimental data of Situ et al. (2005).

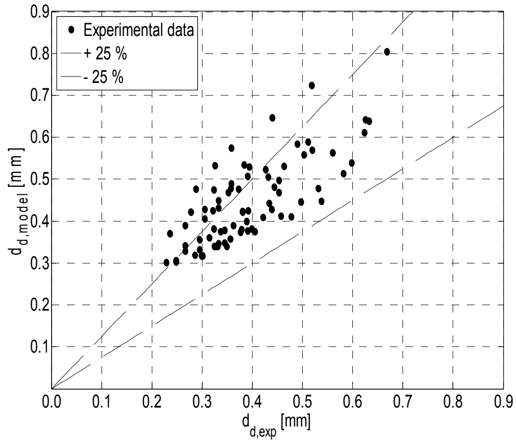

Figure 8: Comparison between model predictions and experimental data of Sugrue (2012).

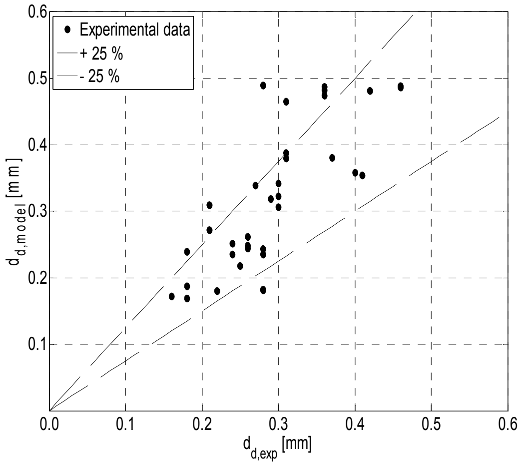

Figure 9 Comparison between model predictions and experimental data of Klausner et al. (1993).

The data from Klausner et al. (1993) for saturated flow boiling of refrigerant R113 allowed further extension of the comparisons, as shown in Figure 9. With an average relative error of 18.9%, the model remains accurate despite the changing fluid and thermal hydraulic conditions. Considering the whole database, the average relative error is satisfactory at 26.7%. A summary of the average relative error for the different datasets and for the database as a whole is provided in Table 2.

Table 2. Summary of the model accuracy for the single datasets and for the whole database.

Data	**Average Relative Error**
Prodanovic et al. (2002)	47.3%
Situ et al. (2005)	24.3%
Sugrue (2012)	19.0%
Klausner et al. (1993)	18.9%
Subcooled boiling	27.4%
Whole database	26.7%

6 Conclusions

An improved mechanistic model of vapour bubble departure in forced convection boiling has been developed. High errors were revealed comparing simple empirical correlations to experiments, suggesting the need for a more mechanistic model. Starting from the model proposed by Klausner et al. (1993), modifications have been included in the surface tension force term and in the equation governing the bubble growth. In the present formulation, the model accounts for the evaporation of the microlayer under the bubble and the heat transfer around the bubble surface. Using the liquid temperature profile calculated from a single-phase temperature wall function scaled on the real wall temperature, regions of superheated and sub-cooled liquid are distinguished and their contributions accounted for separately. An equation governing bubble growth has been validated with some experimental growth transients in sub-cooled water from the work of Prodanovic et al. (2002). Model predictions have been validated against three departure diameter datasets for the sub-cooled flow boiling of water and an additional database of saturated flow boiling of refrigerant R113. The whole validation database guarantees assessment of the model over a wide range of experimental conditions. Good accuracy was reported, with a global average relative error of 26.7%. Higher errors were found only for the dataset of Prodanovic et al. (47.3 %), which proved to be difficult to predict, as found in other studies. In addition, the model predicted well not only data on bubble departure, but also the database of bubble lift-off diameters from Situ et al. (2005). Therefore, the present formulation seems to be able to predict the lift-off diameter after bubble sliding, although further testing is required.

In future, additional validation of the bubble growth model is needed. In particular, accurate quantification of the different contributions from the microlayer, superheating and sub-cooling are required. Additionally, more work is needed to account for bubble shrinking due to condensation, with comparisons of results for other physical parameters, such as the frequency of bubble departure or bubble sliding, also required. Uncertainties still remain in the surface tension force, which has a significant influence on the results for a broad range of data. The development of more accurate and general models for evaluation of bubble contact diameter with the heated wall and contact angles would therefore be useful in improving the overall model accuracy.

Acknowledgements

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Nomenclature

b	parameter / -
C_2	constant / -
C_p	specific heat / J kg^{-1} K^{-1}
D_h	hydraulic diameter / m
d	diameter / m
d_w	bubble-heated wall contact diameter / m
F	force term / N
G	mass flux / kg m^{-2}s^{-1}
h	heat transfer coefficient / W m^{-2} K^{-1}
i	enthalpy / J kg^{-1}
Ja	Jakob number [$\rho_l C_{p,l} (T_l - T_{sat}) / \rho_v i_{lv}$] / -
k	thermal conductivity / W m^{-1} K^{-1}
Pr	Prandtl number [$\mu_l C_{p,l} / k_l$] / -
p	pressure / Pa
Δp	pressure difference / Pa
q''	thermal flux / W m^{-2}
R	bubble radius / m
Re	Reynolds number [$\rho_l U_l d_B / \mu_l$] / -
S	suppression factor / -
T	temperature / K
ΔT	temperature difference / K
t	time / s
U	velocity / m s^{-1}
x	quality / -
y	wall distance / m
y^+	non-dimensional wall distance / -

Greek symbols

α	advancing contact angle / rad
β	receding contact angle / rad
δ	boundary layer thickness / m
θ	channel inclination angle / rad
θ^+	non-dimensional temperature / -
μ	viscosity / Pa s
ρ	density / kg m^{-3}
σ	surface tension / N m^{-1}

Subscripts

B	bubble
c	condensation
conv	convection
d	departure
exp	experimental
l	liquid
lo	lift-off
nb	nucleate boiling
sat	saturation
sub	sub-cooling
tp	two-phase
v	vapour
x	x-direction
y	y-direction

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