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Modeling and Computation of a liquid-vapor bubble formation

Galligo André, Lesage Frédéric, Minjeaud Sebastian

Abstract The Capillary Equation correctly predicts the curvature evolution and the length of a quasi-static vapour formation. It describes a two-phase interface as a smooth curve resulting from a balance of curvatures that are influenced by surface tension and hydrostatic pressures. The present work provides insight into the application of the Capillary Equation to the prediction of single nucleate site phase change phenomena. In an effort to progress towards an application of the Capillary Equation to boiling events, a procedure to generating a numerical solution, in which the computational expense is reduced, is reported.

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1 Introduction

Boiling is a complex phase transitioning process in which a new liquid-vapor interface (bubbles) is created. It is an effective mechanism widely used in energy conversion industrial facilities. However, a precise descriptive/predictive model of bubble formations is needed to better understand its heat transfer characteristics. As an important first step, the question can be addressed from a quasi-static viewpoint. Indeed, at the interface, a classical conservative law governs the surface curvature of the generated bubble. This non-linear law links the difference of pressure and the surface tension effect. After normalization, it can be expressed at each point of the surface by the following equation: $\kappa_1 + \kappa_2 - Bz = \text{constant}$; where B is a Bond number, summarizing the context, z is the elevation and $\kappa_1 + \kappa_2$ is twice the Gaussian mean curvature. Therefore, the study of a growing bubble is amenable to solving geometric computations and non-linear differentiable equation. The main difficulty is to design criteria to detect when the growing bubble will detach from the substrate's nucleation site. Inspired by experimental observations, the second author was able to develop [1, 2] a successful computational strategy. The computational model implemented for the axis-symmetric case (which relies on 2D geometric computations), provides useful information, fully confirmed by experimental observations. Moving forward, we were able to speed up the computations and introduce the use of splines for representing the plane section of the surfaces.

In future work, we will address with similar tools the case for which the nucleation site is on an inclined plane; this geometry better models the one effectively used in industrial plants. Our next target is to better formalize our detachment criteria, in collaboration with an experimental team in Dublin, Ireland; then develop and implement a 3D model for a more general situation. Future studies will also include external stress terms such as cross flows and electrical fields in an effort to move towards realistic and accurate boiling models.

2 Young-Laplace Equation and Capillary Equation

We consider an infinitesimal section of a vapour formation interface defined by two principal radii of curvature in perpendicular planes, as illustrated in Fig. 1.

the problem by imposing a foot radius of unity, in other words the point $(\eta, 1)$ belongs to the curve \mathcal{C} .

The curvature κ_1 is in the $z-r$ plane and the curvature κ_2 is in the plane orthogonal to the tangent unit vector \mathbf{T} . Due to symmetry, the curvatures are equal at the apex origin, they are denoted by $\kappa_0 = \kappa_1 = \kappa_2$. Let g be the gravitational constant and $\Delta\rho$ the difference in density between the two phases, (1) implies the capillary equation:

$$2\sigma\kappa_0 - \Delta\rho gz = \sigma(\kappa_1 + \kappa_2), \quad \text{on } \mathcal{C}. \quad (2)$$

Introducing a dimensionless Bond number, $Bo = \Delta\rho r(\eta)^2 g / \sigma$, we get the adimensionalized form of the capillary equation:

$$2\kappa_0 = \kappa_1 + \kappa_2 + Bo \cdot z, \quad \text{on } \mathcal{C}. \quad (3)$$

2.1 Strategy for Solving the problem

By choosing a parametrization of the curve \mathcal{C} and explicit expressions of the curvatures, the equation (3) can be expressed as a second order Ordinary Differential Equation (ODE) with a free parameter κ_0 (the Bond number being determined by the physical properties of the two fluids). In order to simplify the bubble detachment problem, we decompose the difficulty by fixing a positive value for the parameter η and we consider the corresponding subproblem with the following boundary conditions:

$$(0,0) \in \mathcal{C} \quad ; \quad (\eta,1) \in \mathcal{C} \quad \text{and} \quad \frac{dz}{dr} = 0 \quad \text{at the apex.} \quad (4)$$

Numerical procedures allow to compute a candidate curve solution for each value of the fixed parameter η . Roughly speaking, two boundary conditions are needed to determine the curve from the second order ODE (3) while the third one determines a value for the free parameter κ_0 . So, we obtain a family of curves depending on the parameter η . Then we need a criterion to select the curve that best models the (physical) bubble detachment phenomena. We claim that the detachment profile is identified by noting that at a given height η , below a threshold, one smooth curve satisfies the boundary conditions (4) with at most one inflexion point. This is illustrated in Fig. 2.

The detachment height is then deduced through incremental increases in the parameter to maximize the height η till this property can be satisfied.

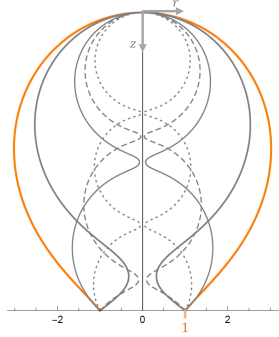


Fig. 2 Set of curves satisfying (3) with the boundary conditions (4) for fixed values of η

2.2 First numerical procedure

This first method is an established approach [1, 3]. The half (smooth) curve \mathcal{C} , is divided in two parts: first a graph of a function $r(z)$ near the apex, then a graph of a function $z(r)$ till the foot. Expressing the curvatures κ_1 and κ_2 in each case, relying on differential geometry formulas, gives rise to a pair of ODEs:

$$2\kappa_0 = \frac{z''(r)}{(z'(r)^2 + 1)^{3/2}} + \frac{z'(r)}{r\sqrt{1 + z'(r)^2}} + Bo \cdot z(r) \quad (\text{ODE1})$$

and

$$2\kappa_0 = \frac{-r''(z)}{(r'(z)^2 + 1)^{3/2}} + \frac{1}{r(z)\sqrt{1 + r'(z)^2}} + Bo \cdot z \quad (\text{ODE2})$$

For each η , we first choose a value of κ_0 . We integrate (ODE1) with the initial boundary conditions $z(0) = 0$ and $z'(0) = 0$. This is done till some value r_1 of r such that $z'(r_1) = 1$. We denote by $z_1 = z(r_1)$. Then we integrate (ODE2)

with the initial boundary conditions $r(z_1) = r_1$ and $r'(z_1) = 1$. This second integration is done until $z = \eta$. The $r(\eta)$ is computed, it will serve for a shooting method. Indeed, performing this process for different values of κ_0 , allows to find a minimum value of κ_0 for which $r(\eta) = 1$.

This numerical approach was successfully implemented using the software Mathematica.

2.3 Second numerical procedure

The half (smooth) curve \mathcal{C} is represented by a kind of arc-length parameterization ($0 \leq t \leq 1$): $r(t), z(t)$ with $|r'(t)|^2 + |z'(t)|^2 = \lambda^2$, depending on a new parameter λ . Again, we can express κ_1 and κ_2 , by similar differential geometry formulas, which provide a system of ODE with respect to the variable t :

$$\begin{cases} 2z'(t)r(t)z''(0) = -\lambda r(t)r''(t) + \lambda z'(t)^2 + Bo\lambda^2 z(t)z'(t)r(t), \\ r'(t)^2 + z'(t)^2 = \lambda^2. \end{cases} \quad (5)$$

The boundary conditions can be expressed as

$$(r(0), z(0)) = (0, 0), \quad (r(1), z(1)) = (1, \eta), \quad z'(0) = 0.$$

Now, we can approximate the functions $r(t)$ and $z(t)$ by cubic spline functions on a subdivision of the interval $(0, 1)$ and express the Boundary Value Problem as a polynomial system of equations, which can be solved by standard techniques. The unknowns of the system are the coefficients of the two splines r and z and the parameter λ .

This second numerical approach was implemented using the software Scilab and is quite efficient since, for a given Bond number, it converges in few iterations of the nonlinear solver. Obviously, the curves obtained by the two numerical methods agree very well. Numerical results obtained with the second approach using a regular subdivision of 50 cells are presented in Fig. 3: at left, for a Bond number equal to 0.0052, the detachment height is estimated to 15.47 whereas at right, for a Bond number equal to 0.047, it is estimated to 7.90.

This second approach is still amenable when we replace the maximization parameter η by the volume of the bubble, an *a priori* more relevant physical quantity. The details will be given in a forthcoming article.

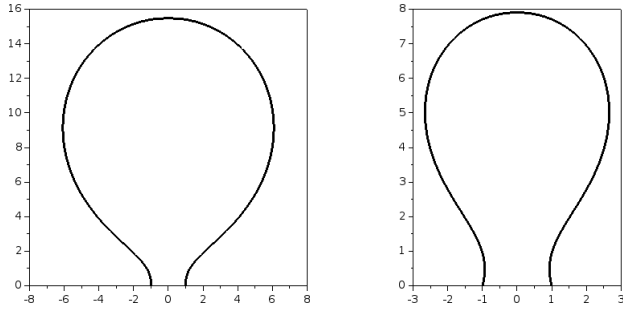


Fig. 3 Numerical solutions obtained for $Bo = 0.0052$ (left) and $Bo = 0.047$ (right)

3 Conclusion

Two numerical methods that solve the capillary equation are reported. The objective of the numerical treatments is to generate curves that model the interface of vapour formations growing from a nucleation site. The first method is an established approach and is used here to provide context and clarity to the solution procedure. The second method is a new refinement to the numerical solution of the Capillary equation. By implementing splines into the procedure, it reduces the computational expense and presents a stepping stone towards more accurate heat transfer predictions of single boiling events.

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