Development and Qualification of Interface-Tracking Model of Boiling in Reactor Coolant Channels

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DEVELOPMENT AND QUALIFICATION OF INTERFACE-TRACKING MODEL OF BOILING IN REACTOR COOLANT CHANNELS

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ABSTRACT

The ability to predict the shape of gas/liquid interfaces is important for various multiphase flow and heat transfer applications [1, 2]. An issue of particular interest to nuclear reactor thermal-hydraulics is concerned with accurate predictions of bubble transport in subcooled boiling. The underlying include: nucleation at the heated wall, bubble transport away from the wall and vapor condensation in contact with subcooled liquid inside the reactor coolant channels.

The purpose of this paper is to present the results of analysis aimed at using first-principle modeling principles based on directly tracking vapor/liquid interfaces to predict bubble shape and velocity evolution in heated fluids at subcooled boiling conditions. The uniqueness of the proposed approach is that a model is shown for the first time, capable of capturing the combined phase-change and kinematic phenomena governing bubble motion across a liquid layer experiencing a sharp temperature gradient from superheated to subcooled conditions. Thus, the effect of simultaneous evaporation and condensation can be investigated on the velocity and shape of vapor bubbles.

The proposed approach is based on a modified level-set method, which has been implemented in the NPHASE-CMFD computer code. The coupled numerical solver can be used to simulate the evolution of gas/liquid interfaces in two-phase flows for a variety of geometries and flow conditions, from individual bubbles to free surfaces (stratified flows) [1, 3]. The emphasis in the present work has been on formulating an accurate computational model capable of capturing the nucleation-driven bubble growth at the wall, combined with a simultaneously occurring condensation at the tip of the bubble which is in direct contact with subcooled liquid. Such situations are particularly important in pressurized nuclear reactors (PWR) where local near-wall boiling may occur at locations along the flow where the liquid subcooling is still quite high.

The issues discussed in the paper include: a description of the novel aspects of the proposed level-set-concept-based method, an overview of the NPHASE code modeling framework and a description of the coupling method between these two elements of the overall model. A particular attention is given to the consistency and completeness of model formulation for the liquid/gas interfacial phenomena corresponding to the coupled evaporation and condensation conditions of heat transfer. Also, the impact of the numerical assumptions and solution method on the accuracy and consistency of predictions will be discussed. The accuracy is measured in terms of the calculated bubble shape and size, and the gas and liquid velocity fields. The results of model testing and validation, including comparisons against analytic solutions for simplified yet physically meaningful situations, are also shown.
1. INTRODUCTION

In the nucleate subcooled boiling mode of heat transfer in heated channels, the wall heat is partially used to form bubbles and the remaining portion is transferred to the liquid. As shown in Figure 1, the heat transfer from the wall in the vicinity of a nucleation site occurs during two distinct periods: the bubble growth time and the waiting time [3].

![Figure 1 - Illustration of the nucleation process at the wall of a heated channel.](image1)

The processes of bubble formation, growth detachment, near-wall flow and collapse in subcooled boiling are shown in Figure 2.

![Figure 2 - Illustration of near-wall bubble history in subcooled boiling. I – low liquid subcooling, II – high liquid subcooling.](image2)

They can be classified as [4]:

- bubble forms at the nucleation site, i.e., an active cavity of a sufficient size,
- the initial growth of a bubble, occurs in the superheated thermal sublayer,
- the top part of the bubble becomes exposed to the subcooled liquid which initiates condensation; also, the bubble may detach from the nucleation site and start sliding along the surface while it is still growing,
- the bubbles can reach their maximum size while being attached to the heated wall or depart from the surface while they are still growing,
- after reaching the maximum size, the bubbles may collapse near the wall or move away from the wall;
- if the subcooling is high and there are many bubbles close together, they will start coalescing and form larger bubbles; this, in turn, may lead to CHF and wall temperature excursion.

It has already been demonstrated that the kinematic phenomena governing the shape and velocity of deformable bubbles in two-phase flows can be numerically simulated using the Level-Set [1, 2] and other interface tracking methods. However, only limited attempts have been made to date to model thermal phenomena between gas/vapor bubbles and the surrounding liquid. In particular, consistent methods of simulating interfacial heat transfer with phase change are yet to be
developed. An example of previous investigations includes the simulations of pool boiling using the Coupled Level Set and Volume of Fluid (CLSVOF) method [5]. However, the emphasis in this work apparently was on the numerical performance (animations) rather than on a discussion of the consistency and accuracy of the methodology itself. Another notable example is the use of the Level Contour Reconstruction [6] method to simulate isothermal film boiling. Because of the isothermal character of the problem, no temperature gradient or phase change occurred at the vapor/liquid interface. Thus, such approach would not be applicable to subcooled boiling.

The purpose of this paper is to present a new state-of-the-art model of bubble growth and/or collapse in the near-wall region of heated channels. The computational implementation of the model is based on combining an incompressible flow model with the Level-Set method [7], both implemented in the NPHASE-CMFD code [8]. The use of incompressible flow assumption combines both advantages and challenges as compared to fully compressible flow models. In fact, except for very special cases, compressible flow models are still not practical to simulate boiling or condensation in two-phase flow systems. On the other hand, the incompressible flow modeling approach require that special numerical solutions be developed to conserve mass and energy accompanying vapor generation and/or collapse, while controlling the pressure and temperature fields inside both liquid and vapor volumes.

As it is shown below, the proposed model in not only capable of modeling the heat transfer and phase change rates at boiling or condensation conditions, but can also be used to simulate simultaneous boiling and condensation at the bubble/liquid interface at conditions corresponding to steep liquid temperature drops from above-saturation to below-saturation over a distance comparable with bubble diameter. To the authors’ knowledge, such situations have never been successively simulated before.

2. MODELING CONCEPT

2.1. Overview of Level-Set Model of Bubble/Liquid Interface Tracking

Interface tracking related equations include the advection equation for the Level-Set function and the Level-Set re-initialization equation [9]. These equations have been incorporated in the NPHASE-CMFD code and coupled with the other governing equations within this code.

_Level-set advection equation_

\[ \frac{\partial \phi}{\partial t} + \nabla \cdot (\tilde{u} \phi) = \frac{\Gamma^*}{\rho_l} \]  \hspace{1cm} (1)

where \( \frac{\Gamma^*}{\rho_l} \) is included to account for the mass transfer when there is phase change. \( \Gamma^* \) is the mass transfer rate per unit area.

_Level-set re-initialization equation_

\[ \frac{\partial \phi}{\partial \tau} = S(\phi_0)(1 - |\nabla \phi|) \]  \hspace{1cm} (2)

where \( S(\phi_0) \) is the sign function.

The above equation is iterated multiple times so that the following condition is satisfied

\[ |\nabla \phi| = 1 \]  \hspace{1cm} (3)
Eq. (3) is required to assure that the level-set function is properly defined as a signed distance function to the interface.

Continuity Equation

\[ \nabla \cdot \mathbf{u} = \Gamma^w \left( \frac{1}{\rho_v} - \frac{1}{\rho_i} \right) \frac{A_{\text{evap}}}{V} \]  

(4)

\( A_{\text{evap}} \) is the phase change interfacial area, and \( V \) is the node volume.

Momentum equation

\[ u_t + \nabla \cdot (\rho u u) = g + \frac{1}{\rho(\phi)} \left\{ -\nabla p + \nabla \left[ \mu(\phi)(\nabla u + \nabla u^T) \right] - \sigma \kappa(\phi) \delta(\phi) \nabla \phi \right\} \]  

(5)

where \( \delta \) is the Dirac delta function. \( \sigma \) is the surface tension. The curvature, \( \kappa \), is calculated as

\[ \kappa(\phi) = \nabla \cdot \left( \frac{\nabla \phi}{|\nabla \phi|} \right) \]  

(6)

2.2. Verification of Incompressible Model of Vapor/Liquid Interface Motion with Phase Change

To test the accuracy of the proposed computational method of predicting phase change due to evaporation and/or condensation at moving liquid/vapor interfaces, a 1-D problem has been formulated with a known analytic solution. The formulation of this 1-D model is illustrated in Figure 3. Liquid flows into the tube from the bottom, vapor is on top of the liquid. Evaporation occurs at the liquid/vapor interface. Inlet velocity of liquid is \( u_{in} \), \( z_i \) is the location of the interface along the z direction. \( 2 \varepsilon \) is the thickness of the interface.

![Illustration of the 1-D Level-set problem with fixed rate of phase change.](image-url)
The following parameters have been chosen: tube length, \( L = 0.2 \) m, \( \epsilon = 6 \) mm, \( P = 6 \) MPa, \( G = 7.58 \) kg/m\(^2\)s, \( v_{in} = 0.005 \) m/s. The initial location of the interface is at \( z_i = 0.05 \) m.

The first three equations describing the liquid, vapor and interface velocities are the continuity, momentum and Level-set equations, respectively

\[
\frac{\partial u}{\partial z} = 0 
\]  
(7)

\[
\frac{\partial u}{\partial t} + \frac{\partial u^2}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g
\]  
(8)

\[
\frac{\partial \phi}{\partial t} + u_i \frac{\partial \phi}{\partial z} = 0
\]  
(9)

The density profile is smoothed along the interface region with the Heavy-side function

\[
\rho(\phi) = \rho_i H(\phi) + \rho_v \left[ 1 - H(\phi) \right]
\]  
(10)

where \( H(\phi) \) is the Heaviside function given by

\[
H(\phi) = \begin{cases} 
1 & \text{if } \phi > \epsilon \\
0 & \text{if } \phi < -\epsilon \\
0.5 \left[ 1 + \frac{\phi}{\epsilon} + \frac{1}{\pi} \sin \left( \frac{\phi}{\epsilon} \right) \right] & \text{if } |\phi| \leq \epsilon
\end{cases}
\]  
(11)

The analytical solution is

\[
u_i = u_i - \frac{G_i}{\rho_i} \left[ \frac{G_i}{\rho_v} + \frac{G_v}{\rho_i} \right]
\]  
(12)

\[
u_i = u_i - \frac{G_i}{\rho_i}
\]  
(13)

\[
\phi(z,t) = -(z - z_i) = -[z - (z_i + u_i t)]
\]  
(14)

The analytical result of the interface location shows that \( z_i(1 \text{ s}) = 0.045 \) m, \( z_i(2 \text{ s}) = 0.04 \) m. The interface is moving backwards against the liquid inlet direction due to a high evaporation rate combined with a low inlet velocity.

The same problem has been encoded in the NPHASE-CMFD code and solved with the Level-Set method to compare with the above analytical solution. It has been found that the numerical results agreed very well with the analytical solution. The calculated location of interface is illustrated in Fig.4.
2.3. Major Computational Issues in the Modeling of Bubble with Phase Change

Several important computational issues have been addressed during the development of a model of vapor bubble experiencing phase change at the interface. These issues include a special treatment of the evaporation term and enthalpy variation in the interface region, and the method of calculating the evaporation term based on a local temperature gradient.

In the Level-Set method, the interface region is an artificial volume adopted to increase the numerical stability of the solver when properties, such as density, change abruptly from liquid to vapor. Besides density, several new variables also require special treatment when phase change is considered. One of the first problems encountered was that an unsmoothed evaporation term in the continuity equation led to large velocity oscillations at the interface region. A smoothed evaporation term was then adopted, which effectively reduced the velocity oscillation. This special treatment also requires a sufficiently large number of nodes within the interface. For instance, the enthalpy at the vapor side of the interface is prescribed as the saturated vapor enthalpy, whereas the enthalpy at the liquid side of the interface is assumed to be equal to the nearest liquid node outside the interface. The purpose of this treatment is to minimize the enthalpy mixing effect near the liquid side of the interface. This effect is mostly numerical and could lead to increased heat transfer between bubble and the surrounding liquid.

A physical conduction term is also needed to properly predict the temperature gradient at the liquid side. This term can be expressed as

\[ Q_{\text{conduct}} = -\frac{k}{C_p} \frac{h - h_f}{\phi} \frac{\Delta V}{\Delta L} \]  \hspace{1cm} (15)

The corresponding evaporation rate term is

\[ \Gamma'' = \frac{k}{c_p} \frac{h - h_f}{\phi} \frac{1}{h_{fg}} \]  \hspace{1cm} (16)

Finally, the numerically solved energy equation becomes
\[
\frac{\partial h}{\partial t} + \nabla \cdot (hu) = \frac{k \nabla^2 h}{\rho(\phi)C_p}
\]  

(17)

3. RESULTS AND DISCUSSION

The results of NPHASE/Level-Set based simulations are shown for two different situations. First, the results for two boiling cases are shown, both dealing with the gravity-driven motion of a vapor bubble surrounded by superheated liquid: a 2-D case and complete 3-D case. Then, a much more complex situation is discussed, when a vapor bubble moves across a liquid field subject to a sharply changing temperature from superheated to subcooled conditions.

In the 2-D Level-Set simulation of evaporating bubble, the computational domain consists of 130 \( \times \) 260 nodes representing a physical domain the dimensions of which are 8mm \( \times \) 16mm. The vapor inside the bubble is at saturation condition under atmospheric pressure, the surrounding liquid is superheated by 10 degrees. As the bubble rises, it also grows due to evaporation at the bubble/liquid interface. Figure 5 shows the temperature contours at different time instants. Note that gravity is pointing to the left in this figure. As can be seen, the bubble grows noticeably as it moves away from the wall. The rising bubble also leaves behind a trail of cooled liquid, forming an interesting shape of the temperature field.

![Temperature profile](image)

Figure 5 - Temperature profile at different time instants, \( ^\circ C \).

Fig.6 shows the velocity vectors at \( t=0.03s \) and \( t=0.06s \), respectively. The density ratio of liquid to vapor is very large under atmospheric pressure, which leads to a high growth rate of bubble volume.
It can also be seen that the rising velocity of the bubble is higher at 0.06s than at 0.03s. This is consistent with the decreasing drag force as the bubble grows.

![Figure 6 - Velocity vector at t=0.03s and 0.06s respectively.](image)

The 3-D evaporation case deals with a vapor bubble rising in a liquid cube. The initial diameter of the bubble was 2mm. The pressure is at 6MPa, the liquid has been initially superheated by 10 degrees to 285.8°C, while the vapor is at saturated temperature of 275.8°C. Figure 7 shows the temperature profile around the bubble at different time instants.

![Figure 7 - Temperature profile of the bubble at different time, °C.](image)
As can be seen, the bubble size did not grow as noticeably as in the previous case because of reduced liquid to vapor density ratio at 6MPa. The shape of the temperature profile behind the bubble is also different from the previous case. This is due to the fact that a 2-D “bubble” displaced more liquid than the spherical bubble in 3-D case, causing a different velocity field around the bubble and thus a different temperature field.

The results for a bubble subject to simultaneous evaporation and condensation are shown in Figure 8. The liquid temperature is a linear function of distance from the heated wall. The highest temperature is 110 °C, the lowest is 90 °C, and the saturation temperature is 100 °C (at atmospheric pressure). As the bubble rises, its volume first grows due to evaporation, then as the surrounding liquid temperature at the front of the bubble drops below the saturation temperature, both evaporation and condensation phenomena occur simultaneously. Fig. 8 shows the temperature profiles at different time instants. As it can be seen, the displacement of the liquid volume behind the rising bubble effectively enhanced the mixing of the liquid temperature near the wall. Fig. 9 presents the evaporation and condensation rates around the bubble. With the bubble rising, the evaporation term becomes smaller, while the condensation effect gradually becomes dominant.

Figure 8 - Temperature profile of the bubble at different time, °C.
4. CONCLUSIONS AND FUTURE WORK

The ability to simulate the growth, condensation and departure of one or multiple bubble using a combined method of CFD and interface tracking technique will have important applications in the research on heat transfer mechanisms in multiphase flows in general, and in nuclear reactors in particular. A new complete model of bubble growth and shrinking under nucleate boiling conditions has been formulated based on the NPHASE-CMFD computer code and the Level-Set interface tracking method. The uniqueness of the new model is in its ability to simulate bubble motion and simultaneous evaporation and condensation across sharply changing liquid temperature fields form superheated to subcooled conditions.

Several computational issues have been addressed and resolved for the first time, regarding the liquid/vapor phase change and its effect on bubble shape and motion, as well as on the liquid temperature field. The results of numerical simulations have been compared against the analytical solution for a 1-D problem, showing excellent agreement. Also, 2-D and 3-D calculations have been performed and the ability of the new model has been demonstrated to simulate the shape evolution and motion of a vapor bubble in a superheated liquid volume. The physically consistency of the model has been shown, including effects such as a decreasing drag force with increasing bubble volume, and a higher volume growth rate under lower pressure.

More work is still needed to generalize the current model, to analyze more complex physical situations encountered in boiling in general, and subcooled boiling in particular, and to perform
further testing and validation studies. Examples include: bubble nucleation and departure from the wall, flow of multiple bubbles, etc. The future research will be important for improving our understanding of nucleate boiling mechanisms and for the development of mechanistic models of sub-cooled boiling in nuclear reactors.

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6. REFERENCES