20th International Conference
NUCLEAR ENERGY FOR NEW EUROPE 2011
Bovec /Slovenia /September 12-15

Quantitative Phase Field Modeling of Boiling Phenomena

Arnoldo Badillo
Paul Scherrer Institute
5232 Villigen PSI, Schweiz
arnoldo.badillo@psi.ch

ABSTRACT

A quantitative Phase Field (PF) model is developed for simulating the dynamic of the liquid-vapor interface during boiling of pure substances. In this model, the interface is described by the variation of a phase indicator field (phase field), which is constant in the bulk phases and varies smoothly across the transition region (diffuse interface). In contrast to sharp interface models, where the velocity of the interface due to phase change depends on the local temperature gradient, the evolution of the phase field follows a relaxation process that minimizes the free energy of the system. The coupling of the phase field equation to the mass, momentum and energy equations allows for quantitative simulations of the interface dynamics. By eliminating the curvature from the phase field equation, the convergence of the model towards the sharp interface limit is no longer controlled by the thermal capillary length, but by the thickness of the thermal boundary layer. With water as the test fluid, simulations of a spherically symmetric bubble growing in a superheated liquid are performed and compared to known analytical solutions and experimental results. Good agreement is found for several superheating levels and saturation pressures.

1 INTRODUCTION

After many years of research, much has been gained on the understanding of boiling, but despite of the efforts put into this enterprise, we are still missing a comprehensive model, able to predict or to incorporate all the relevant physical phenomena involved in this kind of processes. Many questions arise when we think about the fundamental phenomena governing this complex phase change, for example, what is the influence of a force field (like gravity or magnetic field), what are the length and times scales relevant to the dynamic of the interface, what is the relationship between superheating and interface velocity or what are the effects of surface properties. Nowadays, the most advanced models include microscopic phenomena at the contact line and implicit tracking of the liquid-vapor interface during bubble growth [1]. Nonetheless, these models although promising, have not been fully validated and their applicability to polar fluids such as water appears to be a long term goal.

Many models developed for immiscible two phase flows such as Level-Set [2], VOF [3] CIP [4] and sharp interface tracking techniques [5], have shown great accuracy when, for instance, simulating the raising of air bubbles in water [6]. When these models are coupled to the energy equation and a suitable evaporation model is set, it is possible to simulate boiling from a mesoscopic point of view. Under laminar flow conditions, this kind of simulations aims at resolving the smallest time and length scales in the continuum limit, i.e., the interface velocity and thermal boundary layer at the liquid-vapor interface. Ergo these simulations fall into the category of Direct Numerical Simulations (DNS), although this name has commonly

been associated with calculations of turbulent single phase flows, where the smallest length and time scales are established by the dynamics of the smallest eddies.

The resolution of the thermal boundary layer at the liquid-vapor interface is one the most difficult task for any model aiming at mesoscopic simulations (single bubbles). Experiments of bubble growth performed in superheated water at 1 bar, have shown that the thickness of the thermal boundary layer is in the order of tens of microns [7]. This poses a great computational challenge when simulating system sizes in the order of few millimeters. The situation is even more complex when the bubbles are attached to a surface, where microscopic phenomena at the contact line might have an important contribution to the overall evaporation rate [8,9].

Therefore any new model must first be able to predict accurately the growth of unbounded bubbles, where the dominant length scale for the interface dynamics is the thickness of the thermal boundary layer, and then include the effect of a surface. In this work, I present a newly derived Phase Field model for simulating bubble growth in the diffusion-controlled regime.

2 THE PHASE FIELD MODEL

Diffuse interface models are quite popular for two-phase flows simulations and the main reason lies in their simplicity for dealing with complex phenomena such as capillarity and topologic changes of the interface [10]. In these models, the interface is described by a steep but smooth variation of an order parameter or phase indicator field, which keeps a constant value in the bulk phases. This indicator field is then used to model the variation of all the physical properties across the interface. The width of the interface is an arbitrary parameter, often related to the grid spacing, with no physical meaning. By coupling the evolution of the indicator field to conservation laws for mass, momentum and energy, it is possible to solve a unique set of equation to describe the evolution of the bulk as well as the interfacial region, without the need for using any special algorithm for tracking the interface or satisfying sharp interface balances at the interface. Hence, the most complicated part is to find the appropriate source terms in the mass, momentum and energy equations to account for the phase change. For instance, in sharp interface formulations, these source terms do not exist explicitly in the equations, but they are replaced by the so-called jump conditions, which represent conservation laws satisfied at mathematical surfaces.

Phase field models also fall into the smooth interface category, but the path to determine the source terms, which replace the jump conditions, is commonly based on thermodynamic arguments. Simple models of evaporation, like the temperature recovery method [11], allows for calculating the amount of liquid being evaporated based on the local temperature within the diffuse interface, but the time scale on which this process takes place, is somewhat arbitrary. This detail at first glance may appear insignificant, but when performing quantitative simulations, an accurate time scale is absolutely crucial, since the interface dynamic will be primarily dominated by the evaporation rate. Besides, the absorption rate of latent heat by the interface also depends on the time scale we use to evaporate the liquid. In the temperature recovery method, the evaporation rate depends on the amount of superheating at the interface, that is, the amount by which the interface temperature is above its saturation value. When using a source term in the energy equation to account for evaporation, the local temperature inside the interface must decrease due to the cooling effect of evaporation, but at the same time, heat is flowing towards the interface by diffusion. When the evaporation rate equals the heat flux to the interface, we are basically satisfying the Stefan condition, where the interface velocity is proportional to the heat flux at the liquid-vapor interface. Although this model captures the phenomenology of the boiling process, cannot be used to study boiling in the presence of superheated liquid. In a PF approach, the evaporation rate also

depends on the local temperature within the diffuse interface, but the bulk liquid can be superheated and the time scale is determined by an asymptotic analysis of the equations [12]. Furthermore, the evolution of the phase field is not simply based on the amount of superheating at the interface, but also must satisfy the minimization of a functional that represents the free energy of the entire system.

The details behind PF models can be found elsewhere [12, 13], therefore in the following I will only present the main ideas. First, we have to build the free energy functional that represents the free energy of a system in equilibrium, therefore the temperature must be constant everywhere (isothermal system). Cahn and Hilliard [14] proposed a simple (but effective) way to do that; they proposed that the free energy of a point within the system could be expressed as the contribution of a homogeneous part $f_0(\phi)$ (which satisfy classic thermodynamic) and a inhomogeneous part $\lambda|\nabla\phi|^2/2$ accounting for local variations of an order parameter ϕ, thus the free energy of the system is given by

$$F = \int_V \left(f_0(\phi) + \frac{1}{2}\lambda|\nabla\phi|^2 + \cdots \right) dV \tag{1}$$

In the present derivation, the inhomogeneous parameter λ was considered constant. If the system is out of equilibrium, this free energy should be regarded as a snapshot at a given time. In order to move from a non-equilibrium situation to an equilibrium one, the order parameter must change in the direction that decreases the free energy of the system, i.e., the evolution of the order parameter must satisfy the second law of thermodynamics. For a non-conserved order parameter, the evolution of the phase field follows a relaxation process to reach an equilibrium state, which can be expressed mathematically as

$$\frac{\partial\phi}{\partial t} = \frac{1}{\tau}\frac{\delta F}{\delta\phi} = \frac{\mu(\phi)}{\tau} \tag{2}$$

Where τ is the relaxation time, δ is the functional derivative and μ is the transformation potential, which measures the energy difference between equilibrium and non-equilibrium states. Thus, under equilibrium, the transformation potential is zero and no phase change is possible. In order to perform quantitative simulations, equation (2) must be coupled to the mass, momentum and energy equations. To derive the model, we start from a general conservation law

$$\frac{\partial\Phi}{\partial t} = -\nabla\cdot\mathbf{J} + S \tag{3}$$

Where Φ can be a scalar or vector quantity. The flux $\mathbf{J} = \mathbf{u}\Phi + \mathbf{J}_d$ is composed by convective $\mathbf{u}\Phi$ and diffusive $\mathbf{J}_d$ parts and *S* is a source term. Following Sun and Beckermann [15], we consider that the liquid and vapor coexist within the transition region and that each phase has a distinctive mass, velocity and enthalpy (see figure 1). Since the phase field varies continuously from 0 in the vapor to 1 in the liquid, we can make use of this information to find appropriate interpolation functions for all the physical properties and field variables. To obtain the final form of the mass and energy equations, I have used the following definitions

Density: $\rho = \rho_l\phi + \rho_v(1-\phi)$ (4)

Linear momentum: $\rho\mathbf{u} = \rho_l\phi\mathbf{u}_l + \rho_v(1-\phi)\mathbf{u}_v$ (5)

Enthalpy: $H = H_l\phi + H_v(1-\phi)$ (6)

Enthalpy advective flux $H\mathbf{u} = H_l\phi\mathbf{u}_l + H_v(1-\phi)\mathbf{u}_v$ (7)

Solenoidal fields $\nabla\cdot\mathbf{u}_l = \nabla\cdot\mathbf{u}_v = 0$ (8)

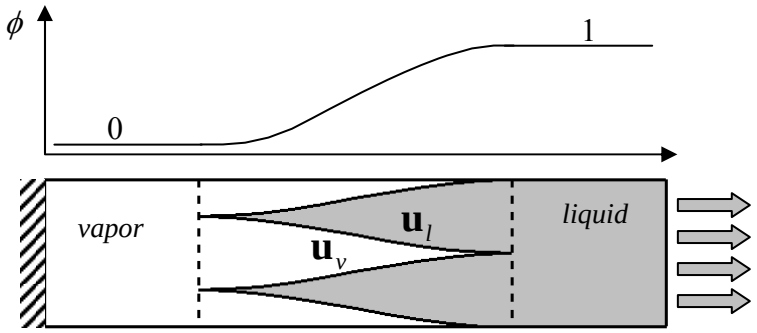

Figure 1. Schematic of the phase distribution within the diffuse interface. The figure also depicts the numerical setup for the "sucking problem".

The details of the derivation of the present model will be presented in a forthcoming publication and only the final set of equations will be written. For the sake of simplicity, I will consider the computational setup depicted in figure 1. In this case, known as the *sucking problem* [16], the velocity of the vapor phase is zero, hence mass conservation states

Mass: $\nabla\cdot(\mathbf{u}_l\phi) = \left(\frac{1}{\rho_l} - \frac{1}{\rho_v}\right)\ddot{\Gamma}$ (9)

Where $\ddot{\Gamma}$ is the mass evaporation rate per unit volume. Since the evaporating liquid suffers a large expansion, a certain amount of mass must leave the system to allow the free movement of the interface. In the case under study, liquid is exiting the system at the right boundary. By neglecting viscous dissipation and considering a quasi-isobaric process, the variation of the internal energy of a differential fluid element is given by the variation of its enthalpy, thus

Energy: $\bar{c}_P\frac{\partial T}{\partial t} + \rho_l^{sat}c_{Pl}^{sat}\mathbf{u}_l\phi\cdot\nabla T = \nabla\cdot(k(\phi)\nabla T + \mathbf{j}_{at}) + \left(L_{sat} - \left(c_{Pl}^{sat} - c_{Pv}^{sat}\right)\Delta T\right)\ddot{\Gamma}$ (10)

The last term in the R.H.S. represents a linearization of the latent heat absorbed during evaporation (or released during condensation). The mixture heat capacity $\bar{c}_P$, thermal conductivity $k(\phi)$ and the phenomenological current $\mathbf{j}_{at}$ are given by

$\bar{c}_P = \rho_l^{sat}c_{Pl}^{sat}\phi + \rho_v^{sat}c_{Pv}^{sat}(1-\phi)$ (11)

$k(\phi) = k_l^{sat}\phi + k_v^{sat}(1-\phi)$ (12)

$\mathbf{j}_{at} = a(\phi)W\left(L_{sat} - \left(c_{Pl}^{sat} - c_{Pv}^{sat}\right)\Delta T\right)\ddot{\Gamma}\mathbf{n}$ (13)

The unusual energy flux $\mathbf{j}_{at}$ is non-zero only within the diffuse interface, and vanishes in the case of equal thermal conductivities and in the sharp interface limit $(W \to 0)$. This current is somehow similar to those proposed by McFadden and co-workers [13] in their version of a phase field model, based on an energy/entropy approach. In their article, they explicitly expressed some concerns about the physical validity of this current, but justified its use as a mean for facilitating computations and modeling. In our model, this current is completely unphysical and appears as a necessity to recover a local thermodynamic equilibrium for artificially enlarged interface thicknesses. As seen in molecular dynamics studies of boiling [17], the real thickness of a liquid-vapor interface is in the range of few angstroms at atmospheric pressure. This ultra-thin interface sets a difficult constraint for any model, due to the fact that there must be several grid points inside the diffuse interface to resolve the derivatives of the phase field. To be able to perform simulations at much larger scales, we must increase artificially the interface thickness to values computationally tractable. In this interface thickening process, some spurious effects are introduced in the energy equation, which have to be balanced by the phenomenological current. Karma [12] proposed a similar expression when deriving a model for dendritic growth, which he called anti-trapping current, thus in resemblance to his idea, I used the subindex ***at.*** The functions entering this current are

$$a(\phi) = \frac{(q(\phi)p(\phi) - \phi)}{\sqrt{2}\phi(1-\phi)} \tag{14}$$

$$p(\phi) = \left(k_v^{sat} / k_l^{sat}\right)\phi \tag{15}$$

$$q(\phi) = \left(k_l^{sat} / k_v^{sat} - 1\right)\phi + 1 \tag{16}$$

In order to close the equations, we have to provide an expression for the transformation potential μ, evaporation rate and relaxation time.

$$\mu(\phi) = W^2\left(\nabla^2\phi - \kappa|\nabla\phi|\right) + 2\phi(1-\phi)(2\phi-1) - 2a_2\phi(1-\phi)(T - T_{sat}) \tag{17}$$

$$\ddot{\Gamma} = \rho_v \mu(\phi)/\tau \tag{18}$$

$$\tau = \sqrt{2}W^2\rho_v^{sat}c_{pv}^{sat} / k_v^{sat} \tag{19}$$

The constant a_2 is defined in the following way

$$\begin{aligned} &I = 0.9428,\ J = 1.3333,\ G = 0.4901\left(k_v^{sat}/k_l^{sat}\right),\ K = 0.1322\left(k_v^{sat}/k_l^{sat}\right) \\ &a_0 = I/J,\ a_1 = (JG - K)/J,\ a_2 = c_{Pv}^{sat}a_0\sqrt{2}/\left(L_{sat}a_1\right) \end{aligned} \tag{20}$$

These constants were determined by an asymptotic analysis of the current model. Details on this kind of analysis can be found in [13].

3 RESULTS

Numerical simulations of single bubble growth in superheated water were carried out at 1 and 0.39 bar. The bubble is assumed to be stationary and therefore the velocity field, due to the liquid expansion, is obtained by direct integration of the mass conservation equation (9). Figure 2, shows the schematic for a stationary bubble with spherical symmetry. A uniform 1D spherical grid with 160 equidistant points was used for both saturation pressures. The system size was 1.5 mm and 9 mm for simulations at 1 and 0.39 bar respectively. The interface thickness was set equal to $W = 1.5\Delta x$ for all the simulations and the physical properties of the fluids were taken from the ASME steam tables. The initial temperature distributions were obtained from Scriven's analytical solution [18].

The interface position predicted by PF simulations was in good agreement with the analytical solution proposed by Scriven for both saturation pressures and superheatings. Nonetheless, it is evident that for small initial bubble sizes, the thermal boundary layer is too thin and clearly under resolved by the mesh. Figure 3a presents the results for two different initial bubble sizes 0.1 mm A and 0.45 mm B. For case A, the correct trend for the interface position is only achieved when the thermal boundary layer is well resolved (at about 4 milliseconds), whereas by setting an initial size of 0.45 mm, the boundary layer is much more thicker than in the previous case, and consequently well captured by the mesh from the beginning of the simulation. This result shows the imperative need for resolving the thermal boundary layer when performing DNS of bubble growth. For water at 0.39 bar, the initial bubble size was 2 mm and the agreement with Scriven's solution is also good.

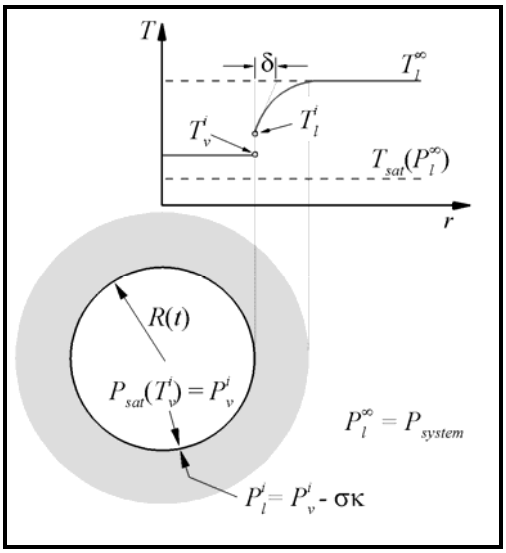

Figure 2. Schematic of the numerical setup used to simulate bubble growth in an unbounded superheated liquid. The figure displays a temperature jump at the interface to illustrate out-of-equilibrium effects such as the interface thermal resistance, which are not considered in the present model.

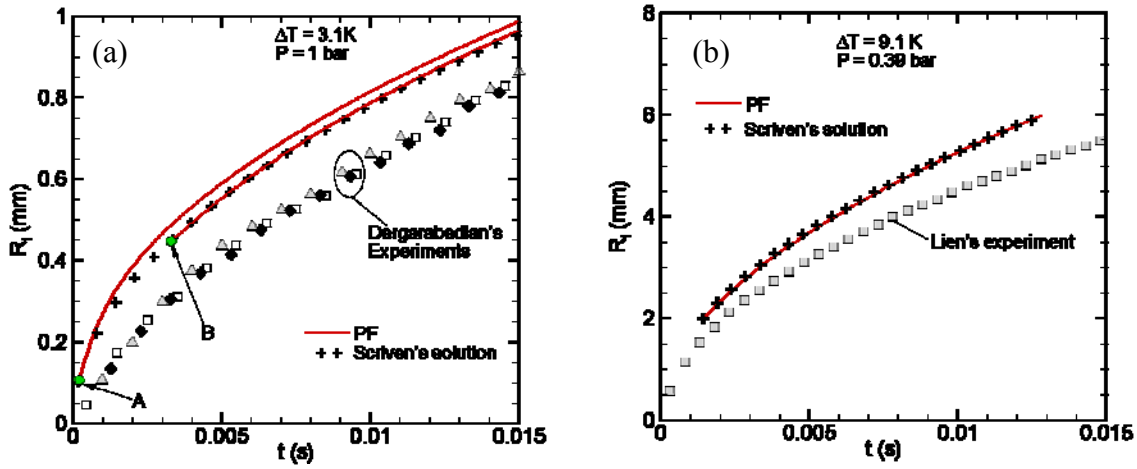

Figure 3. Comparison between predicted and measured bubble size. Red lines represent PF simulations and close symbols correspond to experimental measurements.

Detailed experiments on bubble growth in unbounded systems are extremely scarce and the only experimental data known to me, were obtained by Dergarabedian [7] in 1952 and Lien in 1969 [19]. A comparison between these experimental data and PF simulations shows a fair agreement (see figure 3). For instance, the slope of curve $R_i(t)$ for the two cases under study has the right trend, but the actual bubble size is over estimated. Since the experimental measurements were performed such a long time ago, it was not possible to gather enough information to estimate the level of uncertainty in the bubble size. Nonetheless, since the slope of the curve represents the change of the bubble size (rather than the size itself), its value is assumed to have a lower degree of uncertainty.

The model was also solved in 3D and calculations of bubble growth in water at 10 bar were performed to compare the results with the analytical solution. To speedup the calculations, I took advantage of the spherical symmetry and simulate only 1/8 of the bubble, as seen in figure 4(b,c). The system size was 256 μm^3 and three levels of mesh refinement were used 16^3, 32^3 and 64^3. Bubble size as a function of time is presented in figure 4(a) and the results show a convergent behavior towards the analytical solution.

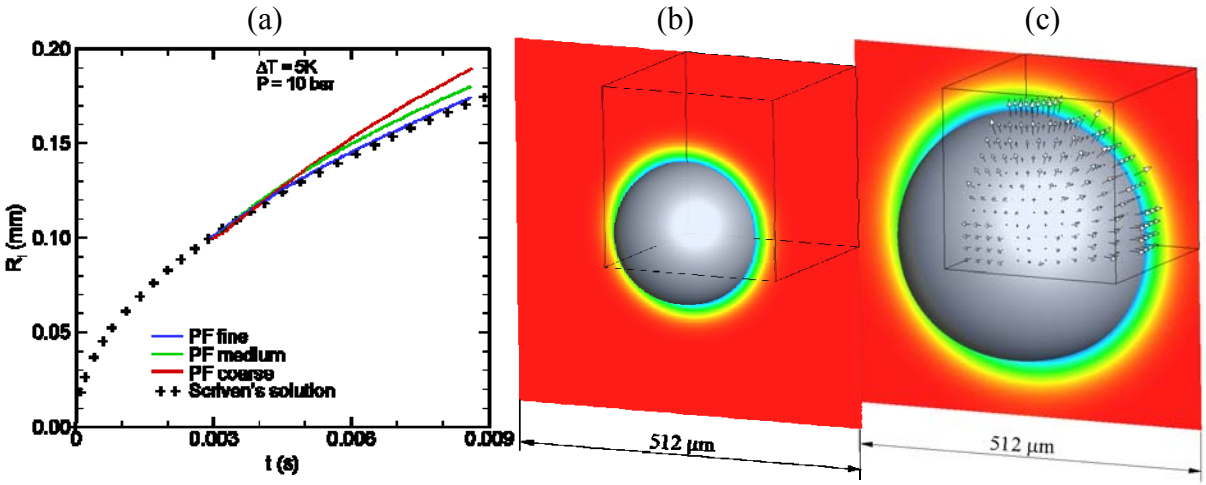

Figure 4: Three dimensional Phase Field simulations of bubble growth. (a) Time evolution of bubble radius, (b) initial condition, (c) final stage of the simulation. Vector field indicates the flow pattern at the liquid-vapor interface generated by the liquid expansion. Color map represents temperature distribution.

Figure 4(b) shows the initial condition for the Phase Field simulations at the finest grid. It can be seen the small extent of the thermal boundary layer compared to the bubble radius, which sets a difficult numerical constraint. In fact, it is the thickness of the thermal boundary layer (not the bubble size) that sets up the scale of the system that is feasible to be simulated.

4 CONCLUSIONS

A newly derived quantitative Phase Field model for simulating liquid-vapor phase transitions has been presented. Comparison with known analytical solutions and experimental data on bubble growth in the diffusion controlled regime, revealed a good performance of the model for different levels of superheating and saturation conditions. The full model, not presented here to comply with space requirements, includes surface tension and coupling with the momentum equations. New numerical results and the full derivation of the model will be presented in forthcoming publications.

ACKNOWLEDGMENTS

The author gratefully acknowledge the financial support from Swissnuclear for the project “Multi-Scale Modeling Analysis of convective boiling (MSMA)”.

REFERENCES

[1] V. Dhir, “Numerical Simulations of Pool-Boiling Heat Transfer”, AIChE Journal, **47**, 2001, pp. 813-834.

[2] W. Olsson. G. Kreiss and S. Zahedi, “A Conservative Level Set Method for two Phase Flow II”, J. Comp. Phys., **225**, 2007, pp. 785-807.

[3] D. Gueyffier, J. Li, A. Nadim, R. Scardovelli and S. Zaleski, “Volume-of-Fluid Interface Tracking with Smoothed Surface Stress Methods for Three-Dimensional Flows”, J. Comp. Phys., **152**, 1999, pp. 423-456.

[4] T. Nakamura, R. Tanaka, T. Yabe and K. Takizawa, “Exactly Conservative Semi-Lagrangian Scheme for Multi-dimensional Hyperbolic Equations with Directional Splitting Technique”, J. Comp. Phys, **174**, 2001, pp. 171-207.

[5] H. Liu, S. Krishnan, S. Marella and H.S. Udaykumar, “Sharp Interface Cartesian Grid Method II: A Technique for Simulating Droplet Interactions with Surfaces of Arbitrary Shape”, J. Comp. Phys., **210**, 2005, pp. 32-54.

[6] Y. Sato, N. Bojan, “A Conservative Local Interface Sharpening Scheme for the Constrained Interpolation Profile Method”, Int. J. Numer. Meth. Fl. (submitted 2011).

[7] P. Dergarabedian, “The Rate of Growth of Vapor Bubbles in Superheated Water”, Ph.D. thesis CALTECH, 1952.

[8] J. Kern and P. Stephan, “Theoretical Model for Nucleate Boiling Heat and Mass Transfer of Binary Mixtures”, J. Heat Trans., **125**, 2003, pp. 1106-1115.

[9] J. Lay and V. Dhir, “Shape of a Vapor Stem During Nucleate Boiling of Saturated Liquids”, J. Heat. Trans., **117**, 1995, pp. 394-401.

[10] Y. Sun and C. Beckermann, “Sharp Interface Tracking Using the Phase-Field Equation”, J. Comp. Phys., **220**, 2007, pp. 626-653.

[11] K. Takase, Y. Ose and T. Kunugi, “Numerical Study on Direct-Contact Condensation of Vapor in Cold Water”, Fusion Eng. Des., **63-64**, 2002, pp. 421-428.

[12] A. Karma, “Phase-Field Formulation for Quantitative Modeling of Alloy Solidification”, Phys. Rev. Lett. **87**, 2001, 115701.

[13] G. McFadden, A. Wheeler and D. Anderson, “Thin Interface Asymptotics for and Energy/Entropy Approach to Phase-Field Models with Unequal Conductivities”, Phys. D., **144**, 2000, pp. 154-168.

[14] J. Cahn and J. Hilliard, “Free Energy of a Nonuniform System. I. Interfacial Free Energy”, J. Chem. Phys. **28**, 1958, pp. 258-267.

[15] Y. Sun and C. Beckermann, “Diffuse Interface Modeling of Two-Phase Flows Based on Averaging Mass and Momentum Equations”, Phys. D, **198**, 2004, pp. 281-308.

[16] S. Welch and J. Wilson, “A Volume of Fluid Based Method for Fluid Flows with Phase Change”, J. Comp. Phys., **160**, 2000, pp. 662-682.

[17] B. Shi and V. Dhir “Molecular dynamics simulation of the density and surface tension of water by particle-particle particle-mesh method”, J. Chem. Phys., **124**, 2006, 204715.

[18] L. E. Scriven, “On the Dynamics of Phase Growth”, Chem. Engng. Sci., **10**, 1959, pp. 1-13.

[19] Y. Lien, “Bubble Growth Rates at Reduced Pressure”, Ph.D. thesis MIT, 1969.