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A New Conservative Phase Change Model for Nucleate Boiling

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ABSTRACT

A new mass-conservative phase change model has been developed for the nucleate boiling simulation. The conservative CIP scheme is used for surface tracking in order to satisfy the mass conservation exactly. As the phase change model, a sharp-interface model is developed, in which the phase change rate can be computed from the heat flux to the interface in a straightforward manner. The developed numerical method is verified for one dimensional phase change problem, and three dimensional bubble growth problem in superheated liquid in unbounded domain. Following these verifications, a saturated nucleate pool boiling simulation is conducted, using a micro region model which can treat the micro physics close to the wall.

1 INTRODUCTION

The Departure from Nucleate Boiling (DNB), the dry-out, and the Critical Heat Flux (CHF) are the key issues in thermal hydraulics with regard to the safety and the efficiency of light water nuclear reactors. In order to study the details of these phenomena and to predict CHF with a numerical simulation, the Computational Fluid Dynamics (CFD) analysis with an interface tracking (IT) method is required instead of using approximated scheme such as the two-phase volume-average model. The long-term goal of our research is to establish a numerical simulation for DNB, dry-out, and CHF within the framework of CFD with IT. In this paper, we focus on the phase change model for nucleate pool boiling.

In the past decade, several phase change models are developed for the level set method [1], the volume-of-fluid (VOF) method [2-3], the coupled level set and VOF method [4], and the front tracking method [5]. These methods are applied for film boiling simulations and nucleate boiling simulations. At present, the level set method developed by Son [1] and VOF by Kunkelmann [6] can simulate the nucleate boiling from a heated wall. However, the level set method is not mass conservative and a special assumption is used in [1]; the vapor is assumed to be the saturation temperature, T_{sat}, for the nucleate boiling while the liquid temperature is T_{sat} for the film boiling. On the other hand, the phase change model in [6] which is originally developed in [3] is not straightforward; the source term for the phase change is artificially smeared out and is shifted across the interface using normalization factors. In this paper, we propose a simple and straightforward phase change model in which the phase change rate computed from the temperature field is directly used as the source term of the volume conservation. The developed model is coupled with a micro region model in order to simulate the nucleate boiling from the heated wall.

The outline of the paper is as follows: in Section 2, the numerical method is described. In Section 3, two cases of verification and a simulation of saturated nucleate pool boiling from heated wall are presented. Finally the conclusions are drawn in Section 4.

2 NUMERICAL METHOD

2.1 Incompressible Navier-Stokes Equations

The equations of momentum and volume conservation, for viscous incompressible flows are written as:

$$\rho\left(\frac{\partial\vec{u}}{\partial t}+\left(\vec{u}\cdot\nabla\right)\vec{u}\right)=-\nabla p+\nabla\cdot\left\{\mu\left(\nabla\vec{u}+\left(\nabla\vec{u}\right)^{T}\right)\right\}+\vec{f}\,,\ \nabla\cdot\vec{u}=\left(\frac{1}{\rho_v}-\frac{1}{\rho_l}\right)\dot{m}\,, \tag{1}$$

where t is the time (s), ρ the density (kg/m^3), $\vec{u}$ the velocity vector (m/s), p the pressure (Pa), μ the viscosity (Pa·s), $\vec{f}$ the body force including the gravity force and the surface tension force, and $\dot{m}$ the phase change rate (kg/m^{3}s). The subscripts v and l denote vapor and liquid, respectively. The continuum surface tension force model [7] is used for the surface tension. The phase change rate $\dot{m}$ is computed with a phase change model and is positive for boiling and negative for condensation.

The governing equations are integrated in time with a projection method, and by a staggered finite volume method in space, on three dimensional Cartesian grids.

2.2 Two phase flow

The color function ϕ is introduced as a volume fraction of the water inside a control volume. The interface between vapor and liquid is defined as iso-surface at $\phi=0.5$. The governing equation for the color function is written as:

$$\frac{\partial\phi}{\partial t}+\nabla\cdot\left(\phi\vec{u}\right)=-\dot{m}\frac{1}{\rho_l}. \tag{2}$$

The CIP-CSL2 method [8] is used for the solution of Eq. (2) in order to achieve the exact volume conservation and the high accuracy for the advection term. For the purpose of preventing smearing out of the color function, the interface sharpening scheme [9] is used.

2.3 Energy Equation

The energy equation is written as:

$$\rho c_p\left(\frac{\partial T}{\partial t}+\vec{u}\cdot\nabla T\right)=\nabla\cdot\left(\lambda\nabla T\right), \tag{3}$$

where c_p is the heat capacity (J/kg), T the temperature (K), and λ the thermal conductivity (W/Km). The temperature of the interface between liquid and vapor is assumed to be T_{sat}. In order to take the interface position into account, the irregular star method is introduced. The finite difference method is used for the cells around the interface, while the finite volume method is used for the other region. Figure 1a shows a sketch of the cells around the interface. The distance between cell center or cell and the interface are written as h. The diffusion term in x-direction of the cell (i,j) is defined in second order accuracy as follows:

$$\lambda_l \left.\frac{\partial^2 T}{\partial x^2}\right|_{i,j} = \lambda_l \left(\frac{2T_{i-1,j}}{h_w\left(h_w+h_e\right)} - \frac{2T_{i,j}}{h_w h_e} + \frac{2T_{sat}}{h_e\left(h_w+h_e\right)} \right). \tag{4}$$

The irregular star method is also used for the convection term, when the temperature gradient ∇T is computed.

2.4 Phase Change Model

We develop the sharp-interface phase change model in which the phase change rate is calculated from the heat flux coming at the interface. The interfacial phase change rate, $\dot{M}$ ($\mathrm{kg/m^2 s}$), is simply defined as $\left(q_{liquid}+q_{vapor}\right)/L$, where q_{liquid} and q_{vapor} are the heat flux coming at the interface from the liquid and the vapor phases, respectively, and L is the latent heat ($\mathrm{J/kg}$). The heat flux q_{liquid} and q_{vapor} are respectively defined as:

$$q_{vapor} = -\lambda_v \nabla T_v \cdot \vec{n}\ ,\ q_{liquid} = \lambda_l \nabla T_l \cdot \vec{n}\ , \tag{5}$$

where $\vec{n}$ is the normal vector of the interface which point from vapor to liquid phase. The schematic sketch of the heat flux is depicted in Figure 1b. The second order accurate scheme is used for the discretization of ∇T to evaluate the heat flux as same order as the diffusion term of the energy equation. When the interface configuration is as depicted in Figure 1a, the x-component of ∇T is discretized as:

$$\left.\frac{\partial T}{\partial x}\right|_{i,j} = \frac{-h_e{}^2 T_{i-1,j} + \left(h_e{}^2 - h_w{}^2\right)T_{i,j} + h_w{}^2 T_{sat}}{h_w h_e \left(h_w+h_e\right)}\ . \tag{6}$$

The phase change rate in unit volume, $\dot{m}$ ($\mathrm{kg/m^2 s}$), is required for the discretization of the phase change rate in the finite volume method. $\dot{m}$ is defined as $\dot{M}\, S_{iso}/V$, where S_{iso} is the area of the interface in a cell, V the cell volume. The area S_{iso} is calculated with the marching cube algorithm [10]. Thus $\dot{m}$ is exactly zero for the cell which does not include interface and the distribution of $\dot{m}$ can be kept sharp.

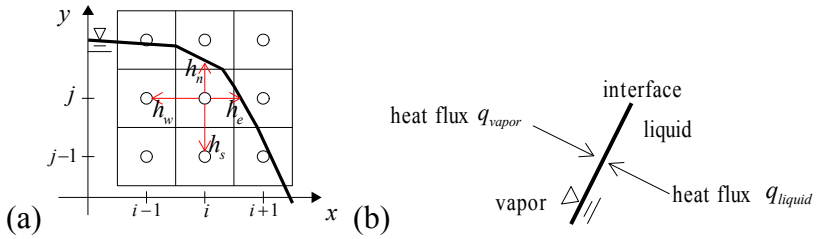

Figure 1: (a) Stencil for irregular star method and (b) heat flux from liquid/vapor to interface.

2.5 Micro Region Model

For the simulation of the nucleate boiling from a heated wall, a special wall boundary treatment is required for the contact line on the wall, since an extremely thin liquid film is formed in the contact line and massive quantities of liquid boils there. Hereafter, we call the

adjacent cell to the wall which includes the contact line "Micro Region Cell" and the other cells "Macro Region Cell".

The analytical model proposed by Stephan and Busse [11] is adopted for the micro region. In this model, fourth order ODE (Ordinary Differential Equations) are derived from two dimensional Navier-Stokes equations and the energy equation. As depicted in Figure 2a, the liquid film thickness δ, the heat flux q_{mic}, and the surface tension force $\vec{f}_{st,mic}$ are obtained as a function of one dimensional position ξ. The solution method proposed by Shikazono [12] is used for the ODE, because we cannot obtain the solution using the boundary condition described in [6, 11].

The computed results of δ and q_{mic} are shown in Figure 2b. The wall temperature is assumed to be constant and is 6.17 K higher than T_{sat}. The contact angle 38° and the curvature 500 m^{-1} is used for the boundary condition at the film thickness of 1.0×10^{-4} m. The dispersion constant is set at 8.5×10^{-21} J which is same as the one used in [13].

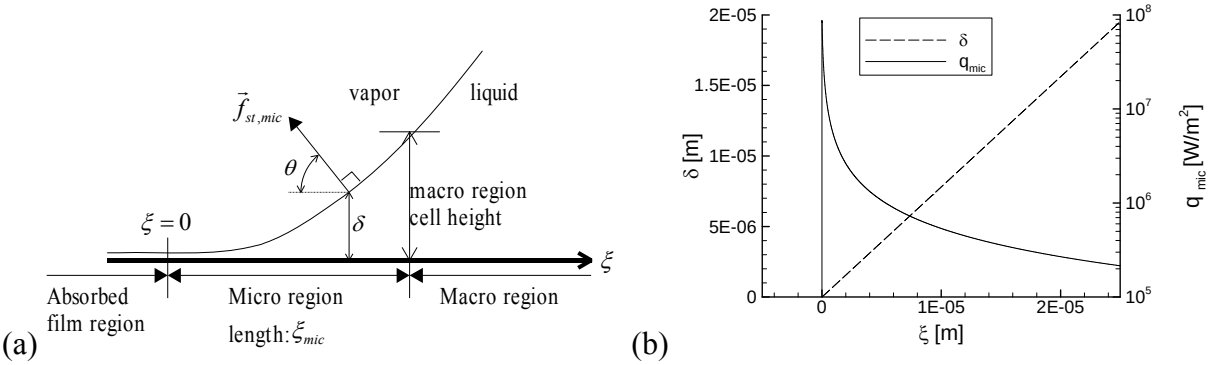

Figure 2: (a) Definition of micro region and (b) computed liquid film thickness and local heat transfer in micro region.

2.6 Coupling of Micro Region Model

The phase change rate and the surface tension force integrated in the micro region model are output for the micro region cell. The phase change rate for the micro region cell is defined as $b\int_0^{\xi_{mic}} q_{mic} d\xi \Big/ L$, where b is the length of the contact line in the micro region cell, ξ_{mic} the length of the micro region. The thickness of the film at $\xi=\xi_{mic}$ is same as the cell height of the macro region as depicted in Figure 2a.

The surface tension force for the micro region cell is defined as: $b\int_0^{\xi_{mic}} \cos\theta \vec{f}_{st,mic} d\xi$, where θ is the angle defined in Figure 2a. Only the tangential component of the surface tension force is transferred to the macro region, since the normal component is balanced with the pressure of the wall.

3 RESULTS OF SIMULATION

3.1 One Dimensional Verification Problem

One dimensional phase change simulation known as the sucking interface problem is conducted as a verification. The problem was originally defined in [2] with the analytical solution and is used for the verification in [6] later. The problem configuration is depicted in Figure 3. The vapor at T_{sat} locates between the wall and the superheated liquid. The liquid boils at the interface resulting from the energy of the superheated liquid. The liquid phase is

pushed to right side due to the volume expansion of the vapor. The analytical solution of the vapor velocity is zero and the liquid velocity is constant in space.

The physical properties used for the simulation are listed in Table 1. The degree of superheat is 5 (K) and the thermal boundary thickness at the initial condition is 4.7×10^{-4} (m). The simulation starts from 0.1 (s) of the analytical solution. The computational domain is set at 0.008 (m). The equal spacing grids are used with four different grid spacing h, the finest grid spacing is 2.5×10^{-5} (m), and the coarsest is 2.0×10^{-4} (m).

Figure 4a shows the distributions of the color function, the phase change rate $\dot{m}$, the temperature T, and the velocity u at time=0.6 (s) for the finest grid. Due to the sharp-interface phase change model, $\dot{m}$ has a value only in a cell which includes interface. Then, the velocity jumps from zero to a certain value in one cell. The vapor temperature is kept at T_{sat} exactly.

The computed interface positions as a function of time are shown in Figure 4b with the analytical solutions. The computed results approach to the analytical solution as the grid spacing becomes smaller and the best agreement is obtained for the finest grid.

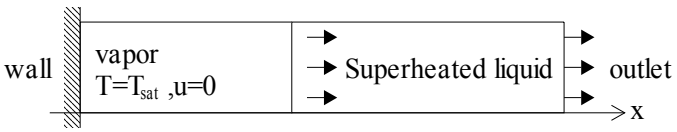

Figure 3: Configuration of sucking interface problem.

Table 1: Physical properties for water/steam at 1 bar.

	ρ, kg/m^3	μ, Pa·s	c_p, J/kg	λ, W/m·K	L, J/kg
vapor	5.79E-01	1.26E-05	2.03E+03	2.50E-02	2.26E+06
liquid	9.58E+02	2.80E-04	4.22E+03	6.79E-01	

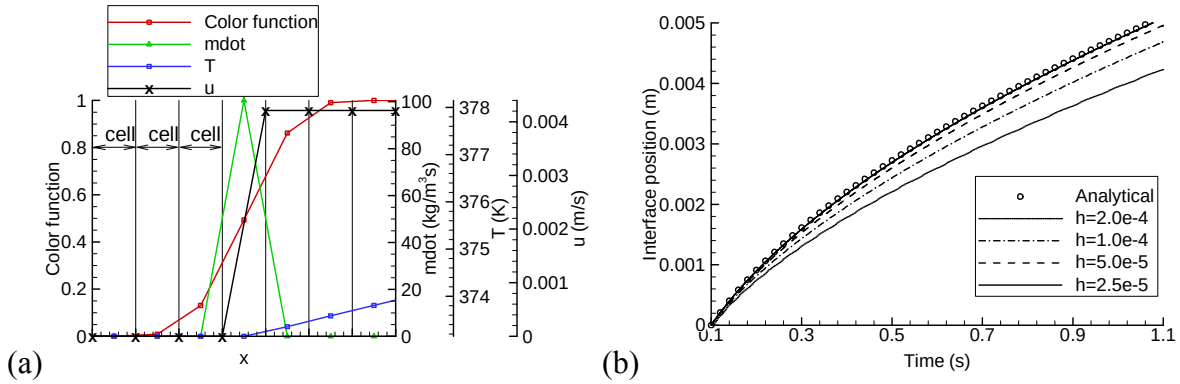

Figure 4: (a) Computed flow field for h=2.5e-5 (m) at time=0.6 (s) and (b) comparison of interface position between analytical solution and computations.

3.2 Bubble Growth in Super-Heated Liquid

As the three dimensional verification of the phase change model, a simulation of the bubble growth in the super-heated liquid is conducted. Here we treat only the heat-transfer-controlled growth; the inertia controlled growth is not taken into account. The working fluids are water and steam at 1 (bar) and the degree of the super-heat is 5 (K). The surface tension coefficient is 0.059 (N/m) and other relevant physical properties are listed in Table 1. The initial condition is taken from the analytical solution [14]; the initial bubble radius is 100 (μm) and the initial thermal boundary thickness is 10 (μm). One eighths of the bubble is computed

using the symmetric boundary condition on the equally spaced Cartesian grid. For the purpose of a grid dependency study, three grid levels are used, the fine grid spacing is 2.0 (μm), the medium 3.9 (μm), and the coarse 7.8 (μm). The computational domain is a 250 (μm) cube.

Figure 5a shows the bubble shape computed with the medium grid. The bubble shape can be kept spherical at time=0.0003 (s). The temperature distribution on the symmetry plane is depicted in Figure 5b with the bubble surface shape drawn with the white line. The temperature inside the bubble is T_{sat} and the relatively thin thermal boundary layer is formed outside of the bubble surface. The computed bubble radius as a function of time is shown in Figure 5c with the analytical solution. The results of computation approach to the analytical solution as the grid spacing decreases. This result indicates that more than five cells are necessary for the thickness of the thermal boundary in this condition.

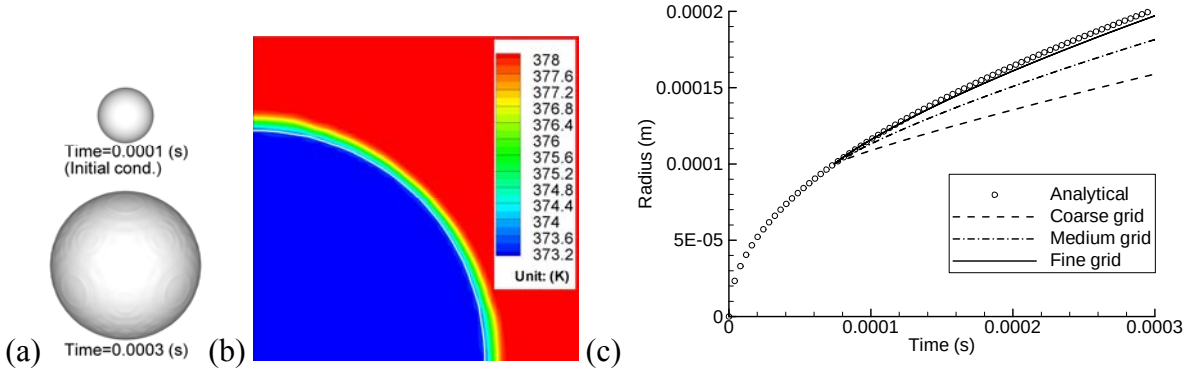

Figure 5: (a) Bubble shape at initial condition and 0.0003 s, (b) temperature distribution on symmetry plane at time = 0.0003 s, (c) comparison of bubble radius between analytical solutions and computations as a function of time.

3.3 Saturated Nucleate Pool Boiling

Three dimensional simulation of the saturated nucleate pool boiling from the heated wall is conducted. The working fluids are water and steam at 1 (bar) and physical properties used for the simulation are listed in Table 1 with the surface tension coefficient 0.059 (N/m). A nucleation site is located at the center of the heated wall. The wall temperature is set at constant which is 6.2 (K) higher than T_{sat}, the contact angle is set at 38°, and the size of the nucleate site is 0.25 (mm). These settings are same as the simulation presented in [1]. The computational domain has dimensions of 8×8×10 (mm) in length, width, and height, respectively. For the purpose of a grid-dependency study, three grid levels are used; the coarse grid spacing is 0.125 (mm), the medium 0.083 (mm), and the fine 0.063 (mm).

The computed flow fields for the medium grid are shown in Figure 6. Following the bubble departure, a new bubble starts to grow from the nucleate site. During the bubble growth, the strong upward flow generated by the volume expansion of the phase change is observed inside the bubble. The high temperature vapor heated on the wall convects upward due to the upward flow. After some degree of the bubble growth, the neck of the bubble starts to shrink due to the surface tension and the bubble finally departs from the wall. The bubble departure diameter and period are 2.4 (mm) and 0.05 (s), respectively while those of the experiments [13] are about 2.1~2.4 (mm) and 0.025~0.033 (s). The reason for the discrepancy of the bubble departure period between the simulation and the experiment is not very clear, but it may be caused by the parameters for the micro region such as the dispersion constant.

Figure 7 shows the computed heat flux and the heat flux generated in micro or macro region as a function of time. Five bubble departures are calculated and the cyclic condition is

obtained for the third and fourth bubble. The deviation of the total heat flux in time is mainly caused by the micro region of which heat flux is proportional to the length of the contact line.

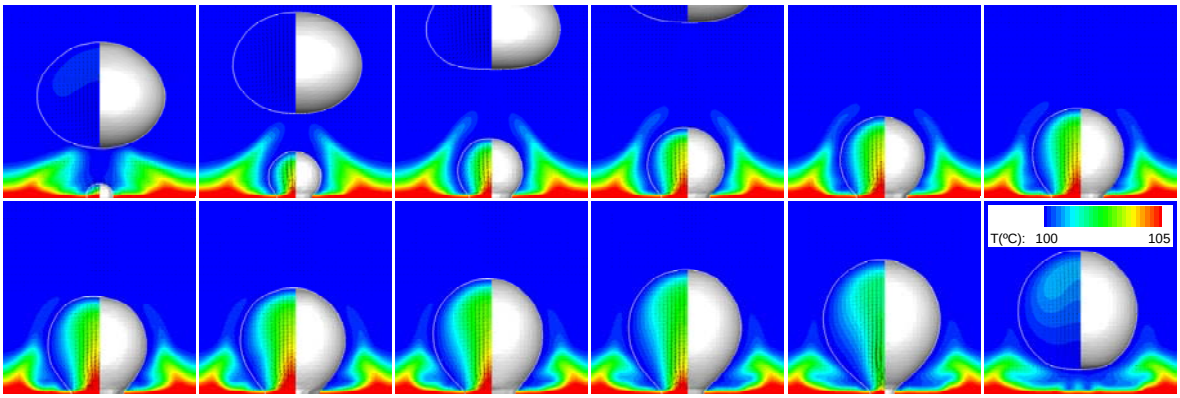

Figure 6: Continuous saturated nucleate pool boiling from heated wall.

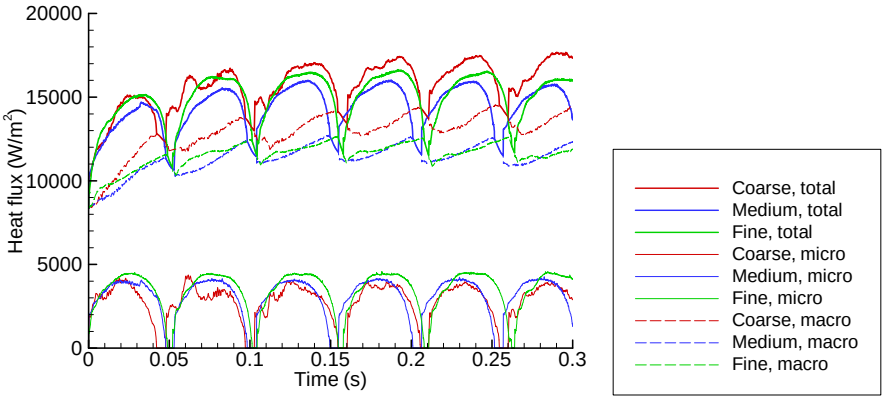

Figure 7: Total heat flux, and heat flux of micro/macro region.

4 CONCLUSIONS

A new conservative phase change model has been developed for nucleate boiling simulations. The model is mass conservative and the phase change model is straightforward; the phase change rate is directly computed from the heat flux to the interface. The computed results of 1D and 3D verification show good agreement with the analytical solutions with the decrease of grid spacing. The simulation of the saturated nucleate pool boiling is conducted and the continuous bubble departure and heat flux can be predicted.

In this paper, the phase change model is coupled with the conservative CIP method. However the phase change model can be coupled with the conservative interface tracking model such as VOF since the phase change model is independent from the interface tracking model.

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