Computations of flows with phase change by implicit coupling of vof method and boundary conditions based on kinetic theory

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Abstract

We developed a practical method for the computation of liquid-vapor two-phase flows accompanied by phase change at the interface. In this paper, we propose an intrinsic improvement by introducing a boundary condition at the non-equilibrium interface, which was derived by Sone and Onishi (Journal of the Physical Society of Japan, Vol.44, (1978), pp.1981-1994.) on the basis of the kinetic theory of gases. The boundary condition, which gives the relationship between the phase change rate and the jump in physical properties, was appropriately integrated with a numerical simulation based on continuum mechanics. The interface was captured by the volume-of-fluid (VOF) method with the piecewise linear interface construction (PLIC) scheme to improve the conservation property of volume. This method was applied to simulating film condensation around a horizontal cylinder. Our results showed that heat and fluid phenomena, including condensation to a liquid film, were successfully reproduced. The order of the spatially averaged Nusselt number on the cylinder was in good agreement with the theoretical value. We compared the results of our method with those of a method that obtains the phase change rate without considering the boundary condition on a molecular scale. We found that our method was effective at simulating film condensation.

Key words : Phase change, Numerical simulation, Multi-phase flow, Kinetic theory of gases, Condensation, Heat transfer

1. Introduction

Fluid flow with phase change is extensively present in industrial applications such as heat exchangers and energy transport processes. Numerical simulations are useful for designing these systems. In this study, we intend to develop a computational method for film condensation.

Many studies have been conducted to develop computational methods for assessing fluid flow with phase change. An interface tracking technique with moving grid was applied to the simulation of boiling flows (Son and Dhir, 1997). On the other hand, the fixed-grid approach can deal with large deformation and geometrical changes of the interface. Yuan et al. (2008) used the volume-of-fluid (VOF) method with an interface reconstruction scheme. Son and Dhir (2008) simulated bubbles with evaporation by the ghost fluid method (Fedkiw et al., 1999) associated with the level-set method. Tomar et al. (2005) employed a coupled level-set and volume-of-fluid (CLS-VOF) method (Sussmann and Puckett, 2005) to simulate film evaporation. In these previous methods, the amount of heat and mass transfer due to the phase change at the interface is determined by a energy balance at the continuum mechanics scale.

Evaporation and condensation phenomena derive intrinsically from molecular interactions at the scale of Knudsen layer in the vicinity of the liquid-vapor interface. These processes have been investigated on the basis of the kinetic theory of gases (Schrage, 1953; Sone and Onishi, 1978; Ytrehus, 1996; Sone, 2002). Some of these studies are concerned

with the analytical descriptions of boundary conditions used with fluid-dynamics equations (Sone, 2002). The boundary conditions derived from these studies have not yet been incorporated into practical two-phase flow simulations based on continuum mechanics in a universal manner.

In our previous study (Ohshima and Kajishima, 2012), we used the boundary condition (Sone and Onishi, 1978) based on the kinetic theory (Sone, 2002) to simulate condensation around a horizontal cylinder. In the method, the phase change rate was given by the difference between the vapor pressure and saturated pressure at the interface. However, because of the assumption about the relationship among pressures (Ward and Fang, 1999; Ward, 2002), which was used for the closure of the governing equations, the scheme was not able to deal with an equilibrium condition without net condensation.

In this paper, we modify our previous method by rearranging the scheme to be applicable even in a static equilibrium state. In the modified method, the boundary condition based on the kinetic theory (Sone, 2002) is implicitly coupled with the VOF method. The boundary condition and an equation that gives the difference in heat flux on both sides of the interface are used to determine the phase change rate. As a practical example, we applied the method to film condensation formed around a heat exchanger tube.

This paper is composed as follows. First, the construction of the computational scheme is explained. Then, the appropriateness of the method is examined by comparing our numerical results to theoretically obtained data on the film condensation. The results are also compared with those obtained by a phase change model that gives the phase change rate without the boundary condition which is based on the kinetic theory.

2. Nomenclature

<u>Roman</u>			
A	heat-transfer area	u_r	radial component of velocity
c	specific heat	u_θ	circumferential component of velocity
D	representative value of length	u_{int}	interface velocity
F	volume fraction	<u>Greek</u>	
g	gravity acceleration	α	intercept of interface
h	heat transfer coefficient	β	coefficient of thermal expansion of water
h_l	specific enthalpy of liquid	Γ	source term
h_v	specific enthalpy of vapor	γ	ratio of the surface area of the interface to the cell volume
$\mathbf{I}$	identity tensor	δ	film thickness
J	Jacobian of coordinate transform	Δt	time increment
k	thermal conductivity	θ	coordinate in circumferential direction
$\mathbf{m}$	normal vector of interface in computational	κ	curvature of interface
$\mathbf{n}$	normal vector of interface	μ	fluid viscosity
$\dot{M}$	total condensation mass flux in the domain	Π	source term
$\dot{m}$	condensation rate of mass per unit time and area	ρ	fluid density
N	number of grid points	σ	surface tension coefficient
p	pressure	Φ	angle from top of cylinder
R	gas constant	Ω	source term
r	coordinate in radial direction	<u>Subscript</u>	
T	temperature	v	vapor phase
T_{int}	temperature of liquid phase at interface	l	liquid phase
t	time	$init$	initial value
T_w	temperature of cylinder surface	int	interface
U	representative value of velocity	w	wall

3. Computational Method

In this study, we considered with film condensation on a cylinder under natural convection. Based on the configuration of the flow field of this simulation, governing equations are written in the two-dimensional polar coordinate system.

3.1. Basic equation

In the VOF method, a density function F ($0 \leq F \leq 1$) is introduced and F is considered as a volume fraction. The volume fraction is defined in each computational cell; $F = 1$ and 0 denote the liquid and vapor phases respectively and the value in between represents the cell which includes the interface. The properties of the fluid occupying each cell are given by volume-weighted arithmetic or harmonic averaging using F as follows:

$$\rho = F\rho_l + (1 - F)\rho_v, \quad (1)$$

$$c = Fc_l + (1 - F)c_v, \quad (2)$$

$$\mu = F\mu_l + (1 - F)\mu_v, \quad \frac{1}{\mu} = \frac{F}{\mu_l} + \frac{1 - F}{\mu_v}, \quad (3)$$

where ρ is the density, c the specific heat and μ the viscosity. Subscripts l and v denote the liquid and vapor phases, respectively. The values of physical properties of each phase are assumed to be constant.

The basic equations of the incompressible flow of a Newtonian fluid are written in the polar coordinate system as follows: equation of continuity

$$\frac{1}{r} \frac{\partial(ru_r)}{\partial r} + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} = \Omega, \quad (4)$$

Navier-Stokes equation

$$\begin{aligned} \frac{Du_r}{Dt} + \frac{1}{\rho} \frac{\partial p}{\partial r} - \frac{u_\theta^2}{r} - \frac{1}{\rho} \left[2 \frac{\partial}{\partial r} \left(\mu \frac{\partial u_r}{\partial r} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left\{ \mu \left(\frac{1}{r} \frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} \right) \right\} \right. \\ \left. + 2 \frac{1}{r} \mu \left(\frac{\partial u_r}{\partial r} - \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} - \frac{u_r}{r} \right) \right] - \frac{\rho - \rho_v}{\rho_l} g \sin \theta + \frac{1}{\rho} f_r = 0, \end{aligned} \quad (5)$$

$$\begin{aligned} \frac{Du_\theta}{Dt} + \frac{1}{\rho} \frac{1}{r} \frac{\partial p}{\partial \theta} + \frac{u_r u_\theta}{r} - \frac{1}{\rho} \left[\frac{\partial}{\partial r} \left\{ \mu \left(\frac{1}{r} \frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} \right) \right\} + \frac{1}{r} \frac{\partial}{\partial \theta} \left\{ \mu \left(\frac{1}{r} \frac{\partial u_r}{\partial \theta} + \frac{u_r}{r} \right) \right\} \right. \\ \left. + 2 \frac{1}{r} \mu \left(\frac{1}{r} \frac{\partial u_r}{\partial \theta} + \frac{\partial u_\theta}{\partial r} \right) \right] - \frac{\rho - \rho_v}{\rho_l} g \cos \theta + \frac{1}{\rho} f_\theta = 0, \end{aligned} \quad (6)$$

equation of internal energy

$$\rho \frac{D(cT)}{Dt} = \frac{1}{r} \frac{\partial}{\partial r} (rq_r) + \frac{1}{r} \frac{\partial q_\theta}{\partial \theta} + \Pi, \quad (7)$$

where g is the gravity acceleration, $\mathbf{f} = (f_r, f_\theta)$ the body force acting on the fluid, and $\mathbf{q} = (q_r, q_\theta)$ the heat flux. Regarding Eq.(7), the frictional heat generation term is ignored. The source terms Ω and Π are the terms attributed to the phase change.

In the cell including the interface, the surface tension, which is evaluated as the body force by the CSF model (Brackbill et al., 1992), is considered as follows:

$$\mathbf{f} = \sigma \kappa \bar{\mathbf{n}}, \quad (8)$$

where σ is the surface tension coefficient, $\bar{\mathbf{n}} = \nabla F / |\nabla F|$ the unit normal vector of the interface to the direction of the liquid phase and κ the curvature of the interface given by following equation:

$$\kappa = \frac{1}{|\mathbf{n}|} \left[\left(\frac{\mathbf{n}}{|\mathbf{n}|} \cdot \nabla \right) |\mathbf{n}| - (\nabla \cdot \mathbf{n}) \right], \quad (9)$$

where $\mathbf{n}$ is the normal vector of the interface to the direction of the liquid phase.

The heat flux $\mathbf{q}$ is evaluated using the effective heat conductivity as follows (Takeuchi et al., 2013):

$$\mathbf{q} = k_n (-\nabla T) \cdot \hat{\mathbf{n}} \hat{\mathbf{n}} + k_t (-\nabla T) \cdot (\mathbf{I} - \hat{\mathbf{n}} \hat{\mathbf{n}}), \quad (10)$$

where k_n and k_t are the effective heat conductivity in the normal and tangential directions of the interface respectively, $\hat{\mathbf{n}}$ the unit normal vector of the interface to the direction of the vapor phase and $\mathbf{I}$ the identity tensor. For the calculation of ∇T of Eq.(10), the representative value T of temperature of the cell is used. For k_n and k_t in Eq.(10), the following mean thermal conductivities are employed (Takeuchi et al., 2013):

$$\frac{1}{k_n} = \frac{F}{k_l} + \frac{1 - F}{k_v}, \quad k_t = Fk_l + (1 - F)k_v. \quad (11)$$

By Eq.(10), in consideration of arithmetic and harmonic mean of thermal conductivity, the heat flux can be determined appropriately depending on the direction of the interface (Takeuchi et al., 2013).

Fig. 1 Physical space and computational space used in this simulation.

3.2. Treatment of liquid-vapor interface with VOF/PLIC

In the VOF method, the advection equation of the volume fraction F on the polar coordinate system is written as

$$\frac{\partial F}{\partial t} + \frac{1}{r} \frac{\partial(rFu_r)}{\partial r} + \frac{1}{r} \frac{\partial(Fu_\theta)}{\partial \theta} = \Gamma, \quad (12)$$

where Γ is the source term that indicates the change in F due to phase change.

Piecewise linear interface construction (PLIC) method (Aulisa et al., 2003) of approximating an interface by linear function is integrated with the VOF method. The PLIC method improves the conservation property of volume. In the method, the interface is approximated by the following linear equation:

$$m_\xi \xi + m_\eta \eta = \alpha, \quad (13)$$

where $\mathbf{m} = (m_\xi, m_\eta)$ is the normal vector of the interface on a computational space, (ξ, η) the computational space and α the intercept of Eq.(13). Although the computational grid is not a rectangular on the physical space, it is uniform square on the computational space after a coordinate transform, that is $\Delta\xi = \Delta\eta = 1$, as shown in Fig.1. For the interface normal vector, the mixed Young-centered (MYC) method (Aulisa et al., 2007) is employed. The volume fraction is advected by using the split Lagrangian explicit method (Aulisa et al., 2007).

3.3. Phase change model

To examine the effectiveness of the proposed model, our results are compared to those obtained from the model which estimates the heat flux from the nearest temperature gradient of the interface without considering the boundary condition by the kinetic theory. We describe the two models in this section.

Considering energy balance at the interface, the condensation rate of mass per unit time and unit area, $\dot{m}$, is given by as follows at the continuum mechanics scale:

$$\dot{m} = \frac{(k_l \nabla T_l - k_v \nabla T_v) \cdot \hat{\mathbf{n}}}{h_v - h_l}, \quad (14)$$

where h_l and h_v are the specific enthalpy of liquid and vapor, respectively. In previous studies on the simulating flows with phase change, Eq.(14) has been widely used to determine the phase change rate (Shirakawa et al., 2000; Onishi et al., 2010; Tanguy et al., 2014). In these studies, the heat flux at the interface is determined based on the nearest temperature gradient. However, rapidly temperature change in the gas phase side occurs in the vicinity of the interface with phase change. Therefore, determining the heat flux by the nearest temperature gradient can cause to increase the difference with an actual heat flux at the interface. In this paper, we propose the method using the temperature jump condition to determine the vapor temperature at the interface in the procedure of calculating the heat flux based on Eq.(14).

To obtain the vapor temperature at the interface, the relation derived by a systematic analysis of the Boltzmann-Krook-Welander (BKW) model (Sone and Onishi, 1978; Sone, 2002)

$$\frac{T_v - T_{int}}{T_{int}} = d_4^* \frac{(\mathbf{u}_v - \mathbf{u}_{int}) \cdot \hat{\mathbf{n}}}{\sqrt{2RT_{int}}}, \quad (15)$$

is introduced, where T_v is the vapor temperature at the interface, T_{int} the liquid temperature at the interface, $\mathbf{u}_v$ the vapor velocity, $\mathbf{u}_{int}$ the interface velocity, R the gas constant of vapor and d_4^* the constant value. For the BKW model,

$d_4^* = -0.44675$ (Sone and Onishi, 1978; Sone, 2002). Using the equation $\dot{m} = -\rho_v(\mathbf{u}_v - \mathbf{u}_{int}) \cdot \hat{\mathbf{n}}$, which gives the relation between $\dot{m}$ and the relative velocity at the interface, Eq.(15) can be rewritten as follows:

$$\frac{T_v - T_{int}}{T_{int}} = -d_4^* \frac{\dot{m}}{\rho_v \sqrt{2RT_{int}}}. \quad (16)$$

The temperature jump given by the kinetic theory of gases Eq.(16) is newly introduced on the model which is based on Eq.(14). Although the vapor temperature at the interface is determined by Eq.(16) in this way, the liquid temperature at the interface is given as estimated value by linear extrapolation. However, the temperature jump, which significantly contributes to the phase change rate, is determined by Eq.(16). In this paper, we call CASE A when this model is used.

As in the model that has been widely used (Shirakawa et al., 2000; Onishi et al., 2010; Tanguy et al., 2014), the condensation rate of CASE B is determined by Eq.(14) without the temperature jump condition of Eq.(16). In CASE B, liquid and vapor temperatures used for the calculations of heat flux at the interface are determined by extrapolation from both sides of the interface. That is, it means to calculate the heat flux using a temperature gradient in the vicinity of the interface. This model, which is integrated on the same numerical scheme with CASE A, is chosen as the comparison to clarify the characteristic of CASE A.

As for the unit normal vector $\hat{\mathbf{n}}$ of Eq.(16), we use following expression in this study:

$$\hat{\mathbf{n}} = \begin{cases} (1, 0) & (m_\xi \geq m_\eta), \\ (0, 1) & (m_\xi < m_\eta). \end{cases} \quad (17)$$

Namely, either direction perpendicular to the cell boundary is determined by the magnitude of values m_ξ and m_η in Eq.(13).

Here, we explain the treatment of temperature and temperature gradient at the interface. Figure 2 shows the treatment of temperature in CASE A and CASE B. Suppose that an interface is given in the j -th cell and values are extrapolated in r -direction. The vapor phase is assumed to be in positive direction of r . The direction for calculation of temperature and temperature gradient is determined in the same way with that of the direction of the unit normal vector in Eq.(17).

In both cases, T_{int} is determined by linear extrapolation using T_{j-1} and T_{j-2} . For the temperature gradient, ∇T_l is given by the gradient of T_{int} and T_{j-1} . Similarly, ∇T_v is calculated as the gradient of T_v and T_{j+1} . In this process, Eq.(16) intervenes to obtain T_v in CASE A.

Fig. 2 Treatment of temperature in the cell including the interface.

The value $\dot{m}$ is considered as the source term in the basic equations. An amount of volume change $\dot{V}$ of liquid and vapor phases, per unit time and unit area, caused by the phase change can be written by following equations, respectively;

$$\dot{V}_l = \gamma \frac{\dot{m}}{\rho_l}, \quad \dot{V}_v = -\gamma \frac{\dot{m}}{\rho_v}, \quad (18)$$

where γ is the ratio of the surface area of the interface to the cell volume $\gamma = S/V$, where V is the cell volume and S the surface area. By mapping the interface on the physical space to the computational space, S is approximated by area of the plane. In this simulation, S is calculated using the coordinate values of the intersections of the equation which represents the interface (13) with the cell boundaries shown in Fig.1. The source term for equation of continuity (4) is as follows:

$$\Omega = \gamma \left(\frac{1}{\rho_l} - \frac{1}{\rho_v} \right) \dot{m}. \quad (19)$$

The change in the internal energy due to the phase change is given as follows in consideration of the latent heat by $\dot{V}_l$ of Eq.(18):

$$\Pi = \gamma(h_v - h_l)\dot{m}. \quad (20)$$

The equation of continuity of homogeneous fluid which is averaged by volume fraction of liquid and vapor phase is given by following equation:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial (r \rho u_r)}{\partial r} + \frac{1}{r} \frac{\partial (r \rho u_\theta)}{\partial \theta} = 0. \quad (21)$$

When an assumption for incompressible fluid $D\rho/Dt = 0$ is considered in Eq.(1), following equation is obtained:

$$(\rho_l - \rho_v) \left(\frac{\partial F}{\partial t} + \frac{1}{r} \frac{\partial (r F u_r)}{\partial r} + \frac{1}{r} \frac{\partial (r F u_\theta)}{\partial \theta} \right) = 0. \quad (22)$$

Equation (4) is considered in Eq.(22), and the source term for advection equation of volume fraction is obtained as follows:

$$\Gamma = \gamma \frac{\rho}{\rho_l \rho_v} \dot{m}. \quad (23)$$

3.4. Outline of computational procedure

The spatial derivative was approximated by the second-order central finite difference with the staggered arrangement of variables. For the time marching, the Adams-Bashforth method was applied to convection and viscous terms in Eqs.(5) and (6) to mitigate numerical instability due to the liquid-vapor density ratio. The second-order Adams-Bashforth method was used as the time marching scheme for the energy equation (7). The procedure to advance a time-increment Δt from the present time step t^n to the next time step $t^{n+1} = t^n + \Delta t$ is summarized as follows:

- (1) The convection and viscosity terms in Eqs.(5) and (6) are calculated using the velocity field and the fluid properties. For these calculations, the values of present and previous time steps (t^n , t^{n-1} and t^{n-2}) are used.
- (2) The condensation rate $\dot{m}$ is determined by Eq.(14) in both cases. In CASE A, Eq.(16) is used to determine T_v of Eq.(14).
- (3) The volume fraction F is updated based on Eq.(12).
- (4) The properties of the fluid occupying each cell in the next time step are determined by Eqs.(1)- (3) and (11).
- (5) By SMAC method, the velocity field of the next time step is obtained through a prediction and correction step. The Poisson equation for the pressure difference is solved by the bi-conjugate gradient stabilized (Bi-CGSTAB) method (Van Der Vorst, 1992).
- (6) From Eq.(7) considering the latent heat of condensation, the temperature field of the next step is determined.

3.5. Computational setup

Fig. 3 Computational domain and computational grid in the case of $N_\theta \times N_r = 240 \times 60$.

Fig. 4 Initial condition of temperature.

Computational domain and a part of computational grid for simulating film condensation on a cylinder in a natural convection field are illustrated in Fig.3. We employed three steps of the grid resolution: namely, the numbers of grid points are $N_\theta \times N_r = 120 \times 30$, 240×60 and 360×120 . The grid spacing is uniform in the circumferential direction and is non-uniform in the radial direction. The spacing in the radial direction becomes smaller towards the cylinder surface. The minimum radial spacing is $0.0031D$ in case of $N_\theta \times N_r = 240 \times 60$. The boundary conditions are also presented in Fig.3. A non-slip boundary condition is imposed at the surface of the cylinder, and a traction-free condition is imposed at the outer boundary of the computational domain. The temperature of the cylinder surface $T_w = 370[\text{K}]$ is kept constant. As an initial condition, a uniform liquid film with a thickness of $\delta_{init} = 0.019D$ at a static state is given on the cylinder. For

Table 1 Computational conditions

Vapor density ρ_v	0.60	kg/m ³
Vapor viscosity μ_v	1.20×10^{-5}	Pa s
Vapor thermal conductivity k_v	2.50×10^{-2}	J/(m K s)
Vapor specific heat c_v	2.05×10^3	J/(kg K)
Vapor specific enthalpy h_v	2.68×10^5	J/kg
Liquid density ρ_l	960	kg/m ³
Liquid viscosity μ_l	3.00×10^{-4}	Pa s
Liquid thermal conductivity k_l	0.675	J/(m K s)
Liquid specific heat c_l	4.22×10^3	J/kg K
Liquid specific enthalpy h_l	4.18×10^5	J/kg
Gas constant of vapor R	461.7	J/kg K
Coefficient of surface tension σ	6.00×10^{-2}	N/m
Density ratio ρ_l/ρ_v	1.60×10^3	-
Viscosity ratio μ_l/μ_v	25.0	-
Thermal conductivity ratio k_l/k_v	27.00	-
Specific heat ratio c_l/c_v	2.06	-

the initial temperature, a layer with a temperature equal to the initial temperature of the liquid phase is given in the vapor phase as shown in Fig.4. It represents the situation that the heat supplied from surroundings is almost going to reach the surface of the liquid film, but the temperature profile is simplified by the step function. To keep the number of stencils for proper extrapolation of vapor temperature at the interface, the thickness of the lower temperature region is set equivalent to the width of the coarsest grid. The blue line in Fig.3 indicates the shape of initial liquid-vapor interface at $r = 0.519D$, and 5 grid points are assigned in the radial direction for the initial liquid film. Similarly, 2.5 and 10 points are assigned to the initial liquid film in cases of $N_\theta \times N_r = 120 \times 30$ and 360×120 , respectively. In Appendix, a preliminary discussion about the influence of the resolution on the temperature profile is summarized.

The values of physical properties and constant used in this simulation are summarized in Table 1. Representative scales are selected as follows: the diameter of the cylinder $D = 0.02$ [m] for the length scale; $U = \sqrt{g\beta(T_{vinit} - T_w)D}$ for the velocity scale and the value is 0.021[m/s] in this case, where $\beta = 7.35 \times 10^{-4}$ [1/K] is the coefficient of the thermal expansion of water at 370[K]; the time is normalized by the characteristic time related to buoyancy $D/U = 0.952$ [s]. The time increment is set to $\Delta t = 5.0 \times 10^{-7}$, which is determined from a viewpoint of numerical stability as to the diffusion and advection terms. Regarding the stability of the diffusion term, Δt needed to be less than $\Delta r^2 \min \rho / (2\mu) = 2.25 \times 10^{-5}$. The maximum Courant number in the computational domain was at around 0.1.

4. Results and Discussion

4.1. Time evolution of flow field and volumetric conservation

Figure 5 shows the time evolution of the shape of the liquid film and the temperature field. The non-dimensional time is defined by $t^* = t/(D/U)$. The liquid film flows along the cylinder and drips off the cylinder. To verify the appropriateness of the proposed method to deal with interface motions with condensation, Fig.6 compares the ratio of the liquid volume in the computational domain E to that obtained through the simulation without condensation. The value of E is defined by following equation:

$$E = \frac{\Sigma JF - \Sigma JF_{init}}{\Sigma JF_{init}}, \quad (24)$$

where J is the Jacobian of the coordinate transformation and ΣJF_{init} the initial volume of the liquid phase. In Fig.6, the dashed lines indicate the results without condensation and the solid lines indicate those with condensation. Three steps of number of grid points $N_\theta \times N_r = 120 \times 30$, 240×60 and 480×120 are examined in each case. When the condensation is not considered, E corresponds to the conservation error of the liquid volume in this simulation.

Without condensation, E of $N_\theta \times N_r = 120 \times 30$ is notably large relative to the other cases before $t^* = 0.04$. The value E then irregularly increase with time because of the liquid dripping. In case of the $N_\theta \times N_r$ is finer than 240×60 ,

Fig. 5 Time evolution of shape of liquid film and temperature field.

the ratios of the error to the amount of condensation are less than 0.01. Thus, the effect of the volume conservation error on the amount of condensation is enough small. This result demonstrated the suitability of VOF/PLIC to considering film condensation in this study.

4.2. Comparison with Nusselt's theory

Our computational results are compared with Nusselt's theory on film condensation. When the temperature at the surface is homogeneous, the spatially averaged Nusselt number $\overline{Nu}_t$ for film condensation on a horizontal tube is theoretically estimated as (Fujii, 2005)

$$\overline{Nu}_t = 0.725 \left(\frac{Ga_D}{H_L} \right)^{1/4}, \quad (25)$$

where Ga_D is the Galileo number defined by $Ga_D = \rho_l^2 g D^3 / \mu_l^2$, H_L the condensation number $H_L = k_l(T_s - T_w) / \{\mu_l(h_v - h_l)\}$ and T_s the saturated temperature $T_s = T_{\text{sat}}$. Equation (25) is derived by the conservation law of energy under the assumption that the liquid temperature at the interface is saturated temperature. However, the relational expression of energy in the vapor phase is not introduced, and the temperature jump is not considered. Although the theoretical background is different with our model, Eq.(25) is used as the reference data for the quantitative comparison with our result.

In order to compare our results to the theoretical value of Eq.(25), we define the Nusselt number $\overline{Nu}$ as spatially averaged over the whole computational domain. Assuming that all of the heat transferred through the interface is used for

Fig. 6 Time evolution of ratio of liquid volume in the computational domain.

Fig. 7 Time evolution of spatially averaged Nusselt number on the cylinder surface. Dashed-line indicates the time average value of $\overline{Nu}$ from $t^* = 0.001$ to $t^* = 0.06$ of each resolution.

phase change, $\overline{Nu}$ is defined as follows:

$$\overline{Nu} = \frac{\bar{h}D}{k_l} = \frac{D}{k_l} \frac{\dot{M}(h_v - h_l)}{A(T_{vinit} - T_w)}, \quad (26)$$

where $\bar{h}$ is the spatially averaged heat transfer coefficient, $\dot{M}$ the total condensation mass flux in the computational domain and A the heat transfer area corresponding to the surface area of the cylinder. In our computational results, we calculated the Nusselt number by using Eq.(26).

In our simulations, noticeable fluctuations of $\overline{Nu}$ were observed actually after $t^* = 0.04$. This is caused by the fluctuation of the condensation rate by the dripping of the liquid film. We focus our attention on the film condensation in this study. Therefore we impose following restrict to exclude the influence of condensation to the dripping liquid; $\dot{M}$ is the amount of condensation in the region of $r/\delta_{init} < 2$.

Figure 7 shows the time evolution of $\overline{Nu}$. During $t^* = 0.03$ and 0.04 in all cases, $\overline{Nu}$ takes maximum value. It is related to liquid dripping. As shown in Fig.7, noticeable oscillations of $\overline{Nu}$ are observed during $t^* = 0.02$ and 0.04 in the cases of $N_\theta \times N_r = 240 \times 60$ and 480×120 . These oscillations are caused by the extrapolation in the phase change model because the wavenumber increases with the number of grid points. According to Eq.(26), oscillations of $\overline{Nu}$ are directly derived from those of the condensation rate. The condensation rates fluctuate because the temperatures defined

Fig. 8 Time evolution of distance from the cylinder surface to the interface position (film thickness). Φ is angle from the top of the cylinder. Dashed-line indicates the line of $\delta/\delta_{init} = 2$.

at different cells are used for extrapolation when the interface crosses the cell boundary. However, since a significant difference is not observed among all cases of time-averaged $\overline{Nu}$ as shown in Fig. 7, the fluctuations do not give significant influences on $\overline{Nu}$.

As shown in Fig.7, the order of $\overline{Nu}$ are in good agreement with the theoretical value. However, $\overline{Nu}$ is smaller than the theoretical value in the same order. Therefore the effect of considering the temperature jump becomes obvious as the difference of Nusselt number as shown in Fig.7.

For the time-averaged values of $\overline{Nu}$ indicated in Fig.7, there is no significant difference among the three conditions of resolution. However, the conservation error shown in Fig.6 is relatively large in the case of $N_\theta \times N_r = 120 \times 30$. Also, as shown in Appendix, the resolution should be finer than $N_\theta \times N_r = 240 \times 60$ by examining the influence of the resolution on the thermal boundary. Therefore, the number of grid points should be more than $N_\theta \times N_r = 240 \times 60$ in this study. Namely, there should be more than 5 grid points for the initial liquid film.

Figure 8 shows the time evolution of the film thickness as a function of Φ in the case of $N_\theta \times N_r = 240 \times 60$. About 12 cells are arranged in the radial direction between the cylinder surface and the position $\delta/\delta_{init} = 3$. Even after $t^* = 0.04$, the film is thinner than $2\delta_{init}$ in the region that Φ is 165[deg] or less. According to the restriction on $\dot{M}$, therefore, the region excluded from the estimation of $\overline{Nu}$ is restricted to more than 165[deg].

To examine a factor of change in the Nusselt number, Fig.9 shows the time evolution of temperature profiles in the case of $N_\theta \times N_r = 240 \times 60$. As typical points where the film condensation occurs, Fig.9 shows the profiles of the positions of at $\Phi = 45$ and 135[deg]. Figure 9 shows the monotonic change with time in the temperature and temperature gradient. The temperature gradient changes more notably with time in $r/D = 0.55 - 0.6$ compared with the change in the closer region $r/D < 0.55$ to the interface. The time evolution of temperature gradient observed in Fig.9 shows that the temperature field is in transient state by the development of liquid film with condensation. According to Eqs.(14) and (26), the condensation rate and $\overline{Nu}$ are affected dominantly by the temperature gradient. However, the monotonic change in the $\overline{Nu}$ with time is not observed as shown in Fig.7. Therefore, the condensation rate and the $\overline{Nu}$ are affected significantly by the temperature at the interface, and the influence of the temperature field by the development of the liquid film as shown in $r/D = 0.55 - 0.6$ in Fig.9 is small.

4.3. Comparison with the phase change model without temperature jump condition

Figure 10 shows the time evolution of $\overline{Nu}$ in CASE B. The value $\overline{Nu}$ in CASE A is also presented in Fig.10. The difference of $\overline{Nu}$ between two cases becomes smaller with time. But $\overline{Nu}$ is noticeably large compared to that in CASE A at the initial stage and is larger about 2.6 times than the theoretical value at the maximum. This is because the initial temperature have more significant influence. In CASE B, the temperature jump based on the kinetic theory is not considered in the phase change models, whereas the condensation rate in CASE A is given by Eqs.(14) and (16). In CASE B, the condensation rate is more significantly affected by the temperature other than the interface though the condensation rate intrinsically determined by the temperature jump according to Eq.(16) of molecular scale. Therefore the difference

Fig. 9 Time evolution of radial temperature profile at $\Phi = 45$ and 135 [deg].

Fig. 10 Time evolution of spatially averaged Nusselt number on the cylinder surface.

of $\overline{Nu}$ between the results in both cases becomes large, and the difference between the theoretical value becomes larger in comparison with that in CASE A. Thus, the model of CASE A estimates the condensation rate more appropriately considering the effect of the kinetic theory.

5. Conclusions

A computational method, which considers the effect of a non-equilibrium at the interface based on the kinetic theory, for flows with phase change was proposed. In this method, the boundary condition which gives the relationship between the condensation rate at and the temperature jump on a molecular scale was implicitly coupled with the VOF method. A phase change model, which has been widely used so far, decides the phase change rate so as to satisfy the energy balance at the interface. In the proposed model, the temperature jump condition by the kinetic theory is introduced to the equation of energy balance at the interface. This model is also applicable to flows with evaporation in principle. In this study, as a first step to develop a universal phase change model, the proposed method was applied to the film condensation around a cylinder.

The order of the Nusselt number of our results were in good agreement with the theoretically estimated value. At the same time, a difference in the Nusselt number of the same order between our results and the theoretical value was found. The theoretical background is different between Nusselt's theory and our model, and one of the causes of the

difference is to introduce the temperature jump by the kinetic theory in our model. In addition, our results were compared with those obtained from the phase change model without the jump condition. As a result, our model estimated the phase change rate more appropriately on the basis of the temperature jump condition. In the model without the jump condition, the condensation rate is more strongly affected by the temperature other than the interface. Therefore we think that the proposed model, which reduces the influence of the temperature other than the interface, can predict the phase change rate more appropriately in more extensive condition on non-equilibrium at the interface. Also, the results of this study showed that our method can be potentially used for quantitative prediction of film condensation.

Appendix: Preliminary discussion about the computational grid and the thermal boundary.

In general, when a resolution become fine, the computational results of differential equation become closer to the solutions of equation depending on order of accuracy. In this simulation, however, the influence of numerical behavior, when the values at the interface are extrapolated using the values at discretized points, is large. Therefore, when the interface crosses the cell boundary, the extrapolated values might fluctuate. This problem is not necessarily improved by using finer grid. Therefore, to clarify systematically including the influence of factors other than the accuracy order is difficult. However, it is crucial to consider the influence of the resolution, and we examined the influence of resolution by evaluating the temperature profile.

Fig.11 shows the temperature profile in radial direction at $\Phi = 45[\text{deg}]$ at $t^* = 0.04$. The thermal boundary layers on temperature were in $r/D = 0.51$ to 0.65 in all cases. The temperature profiles were in good agreement in two cases of $N_\theta \times N_r = 240 \times 60$ and 480×120 . Thus, we think that the number of grid points $N_\theta \times N_r = 240 \times 60$ is enough for our simulation. In this case, about 18 grid points are in the thermal boundary layer in the radial direction shown in Fig.11.

Fig. 11 Temperature profile near the interface at $\Phi = 45[\text{deg}]$.

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