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journal homepage: www.elsevier.com/locate/ichmtDevelopment of a vapor–liquid phase change model for volume-of-fluid method in FLUENT[☆]Dong-Liang Sun^a, Jin-Liang Xu^{b,*}, Li Wang^c^a State Key Laboratory of Alternate Electrical Power System with Renewable Energy Sources, North China Electric Power University, Beijing 102206, China^b Beijing Key Laboratory of Energy Safety and Clean Utilization, North China Electric Power University, Beijing 102206, China^c Beijing Key Laboratory of Multi-Phase flow and Heat Transfer of Low-Grade Energy, North China Electric Power University, Beijing 102206, China

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ABSTRACT

In this paper, a vapor–liquid phase change model is proposed for volume-of-fluid (VOF) method in FLUENT. This model is suitable for the case in which both unsaturated phase and saturated phase are present. In this model: (1) the unsaturated-phase thermal conductivity λ_{uns} and specific heat $C_{p,uns}$ are actual physical parameters; (2) the saturated-phase thermal conductivity λ_s and specific heat $C_{p,s}$ are assumed as zero and $C_{p,uns}$, respectively; (3) the interfacial mass-transfer rate $\dot{m}_s = -\dot{m}_{uns} = 2\lambda_{uns}(\nabla\alpha_{uns}\cdot\nabla T)/L$. Finally, the accuracy of the vapor–liquid phase change model is verified by one-dimensional Stefan problem and two-dimensional film boiling problem.

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1. Introduction

Two-phase flow problems could be found in many industrial processes. But it is a great challenge to simulate these problems accurately. In the few decades, many moving interface tracking methods have been developed to simulate complex two-phase flow problems. And the most important ones include the front tracking method [1], the marker particle method [2], the level set (LS) method [3,4] and the volume-of-fluid (VOF) method [5,6]. FLUNET is the world's most widely used CFD software. The VOF method has been employed in FLUENT to simulate two-phase flow with a free surface. However, the accurate vapor–liquid phase change model is still unavailable.

In the existing models, the vapor–liquid phase change model proposed by Lee [7] has been most widely used. Its expressions are shown below:

$$\dot{m}_v = -\dot{m}_l = r\alpha_l\rho_l \frac{T - T_{sat}}{T_{sat}}, \quad T > T_{sat} \text{ (boiling process)} \quad (1)$$

$$\dot{m}_l = -\dot{m}_v = r\alpha_v\rho_v \frac{T_{sat} - T}{T_{sat}}, \quad T < T_{sat} \text{ (condensation process)} \quad (2)$$

where r stands for mass-transfer intensity factor with unit s^{-1} . Being of an empirical coefficient, r is given with different values for different problems. De Schepper et al. [8] adopted this model to simulate the flow boiling process of a hydrocarbon feedstock in the tubes of a convection section heat exchanger of a steam cracker. Here, r was set as

0.1. Alizadehdakheel et al. [9] chose the same value, 0.1, to study the evaporation and condensation phenomena in a thermosyphon. However, in the references [10] and [11] r was set to be 100.

Interfacial temperature is usually set as saturation temperature in the phase change process. Based on Fourier's law, the interfacial heat flux jump can be calculated by the following expression.

$$\|\vec{q}_i\| = \left[\left(-\lambda_l \frac{\partial T}{\partial n} \Big|_l \right) - \left(-\lambda_v \frac{\partial T}{\partial n} \Big|_v \right) \right] \vec{n} \quad (3)$$

where \vec{n} is the interfacial unit normal vector and points toward the vapor phase.

In References [12] and [13], the following vapor–liquid phase change model was derived according to Eq. (3).

$$\dot{m}_v = -\dot{m}_l = \frac{(\alpha_v\lambda_v + \alpha_l\lambda_l)(\nabla\alpha_l\cdot\nabla T)}{L} \quad (4)$$

because of unreasonable assumptions in the process of derivation, there is a large deviation between the computational results and the actual physical phenomena. For example, the bubble growth rate is not relevant to the vapor thermal conductivity λ_v in the growing process of saturated bubble in superheated liquid. However, Eq. (4) contains the information of λ_v , which does not match the actual physical process.

Based on the VOF method, many authors have developed the program codes for solving the phase change problems, such as Welch and Wilson [14] and Guo et al. [15]. The key point of these methods is how to accurately calculate the interfacial heat flux on both sides, ie. $-\lambda_l\partial T/\partial n|_l$ and $-\lambda_v\partial T/\partial n|_v$ in Eq. (3). These methods can simulate the boiling and condensation problems accurately. However, the

[☆] Communicated by P. Cheng and W.Q. Tao.

* Corresponding author.

E-mail address: xjl@ncepu.edu.cn (J.-L. Xu).

Nomenclature	
C_p	specific heat
F_V	interface-induced volume force
g	gravity acceleration
Gr	Grashof number,
h	apparent energy with the zero defined at 298.15 K
L	latent heat
\dot{m}	interfacial mass-transfer rate
\vec{n}	interfacial unit normal vector
Nu	Nusselt number
p	pressure
Pr	Prandtl number
$\ \vec{q}_i\ $	interfacial heat flux jump
q_v	volume heat quantity
r	mass-transfer intensity factor
S_h	heat source term due to phase change
t	time
T	temperature
v	velocity
x, y	coordinates
<i>Greek symbols</i>	
α	volume fraction
δ	interface position
δx	cell width
κ	interface curvature
λ	thermal conductivity
λ_0	unstable Taylor wavelength
λ	characteristic length
μ	dynamic viscosity
ρ	density
σ	surface tension coefficient
<i>Subscripts</i>	
i	grid point
l	liquid phase
I	interfacial surface
s	saturated phase
sat	saturated temperature
uns	unsaturated phase
v	vapor phase
V	volume
w	wall

solving process is complicated and needs to acquire interfacial positions and other information near interfaces. So it is very difficult to extend these methods to FLUENT.

In this paper, a vapor–liquid phase change model is proposed for volume-of-fluid (VOF) method in FLUENT. This model is suitable for the case, in which one of the two phases is unsaturated phase, i.e. under supercooled or overheated condition, the other is saturated phase, i.e. under saturation temperature. In the following we will introduce this model for incompressible two-phase flow and heat transfer in details.

2. Governing equations

VOF method was developed by Hirt and Nichols [5] in 1981. A volume fraction α , of which the value lies between 0 and 1, is defined in this method. In each control volume, the volume fractions of all phases sum to unity.

$$\alpha_s + \alpha_{uns} = 1 \quad (5)$$

where the subscripts s and uns denote, respectively, the saturated and unsaturated phases.

The volume fraction equations of saturated and unsaturated phases can be written as

$$\frac{\partial \alpha_s}{\partial t} + \nabla \cdot (\vec{v} \alpha_s) = \frac{\dot{m}_s}{\rho_s} \quad (6)$$

$$\frac{\partial \alpha_{uns}}{\partial t} + \nabla \cdot (\vec{v} \alpha_{uns}) = \frac{\dot{m}_{uns}}{\rho_{uns}} \quad (7)$$

where $\dot{m}_s = -\dot{m}_{uns}$.

Momentum equation:

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot [\mu (\nabla \vec{v} + \nabla \vec{v}^T)] + \rho \vec{g} + F_V \quad (8)$$

where

$$\rho = \rho_s \alpha_s + \rho_{uns} \alpha_{uns} \quad (9)$$

$$\mu = \mu_s \alpha_s + \mu_{uns} \alpha_{uns}. \quad (10)$$

Surface tension is a surface force, which is converted into a volume force F_V by the continuum surface force (CSF) model developed by Brackbill [16]. F_V can be written as

$$F_V = \sigma \frac{\alpha_s \rho_s \kappa_s \nabla \alpha_s + \alpha_{uns} \rho_{uns} \kappa_{uns} \nabla \alpha_{uns}}{0.5(\rho_s + \rho_{uns})} \quad (11)$$

where σ and κ denote the surface tension coefficient and the interface curvature, respectively. The interface curvature is obtained from

$$\kappa_s = -\kappa_{uns} = -\nabla \cdot \left(\frac{\nabla \alpha_s}{|\nabla \alpha_s|} \right). \quad (12)$$

Energy equation:

$$\frac{\partial}{\partial t} (\rho h) + \nabla \cdot (\rho \vec{v} h) = \nabla \cdot (\lambda \nabla T) + S_h \quad (13)$$

where

$$h = \frac{\alpha_s \rho_s h_s + \alpha_{uns} \rho_{uns} h_{uns}}{\alpha_s \rho_s + \alpha_{uns} \rho_{uns}} \quad (14)$$

$$h_s = C_{p,s}(T-298.15), h_{uns} = C_{p,uns}(T-298.15) \quad (15)$$

$$\lambda = \lambda_s \alpha_s + \lambda_{uns} \alpha_{uns} \quad (16)$$

$$S_h = \begin{cases} -\dot{m}_s L & \text{when saturated phase is vapor phase} \\ \dot{m}_s L & \text{when saturated phase is liquid phase} \end{cases} \quad (17)$$

3. Phase change model

In this section, a vapor–liquid phase change model is proposed for the volume-of-fluid (VOF) method in FLUENT. This model is suitable for the case in which both unsaturated phase and saturated phase are present. It includes the following three part contents:

Content-1: The unsaturated-phase thermal conductivity λ_{uns} and specific heat $C_{p,uns}$ are actual physical parameters.

Content-2: The saturated-phase thermal conductivity $\lambda_s = 0$ and specific heat $C_{p,s} = C_{p,uns}$. The saturated-phase temperature equals saturated temperature everywhere and there does not exist heat conduction, so λ_s is assumed as zero. Because of the temperature unchanged, the value of $C_{p,s}$ has no effect on the calculation results. For the convenience of calculation, $C_{p,s}$ is assumed to equal $C_{p,uns}$.

Content-3: Solve the interfacial mass-transfer rate \dot{m} . Because one phase is saturated in this model, Eq. (3) can be rewritten as

$$\|\vec{q}_I\| = \left(-\lambda_{uns} \frac{\partial T}{\partial n} \Big|_{uns} \right) \vec{n} \quad (18)$$

where \vec{n} points toward the saturated phase.

$\|\vec{q}_I\|$ is heat flux jump at interfacial surface with unit $w \cdot m^{-2}$. Similar with the CSF model, the interface is interpolated as a transient region with a finite thickness. $\|\vec{q}_I\|$ is converted into a volume heat quantity with unit $w \cdot m^{-3}$, which is written as

$$\|\vec{q}_I\| = \int_{-l}^l q_V d\vec{l} \quad (19)$$

where \vec{l} points toward the saturated phase. Assume that the unsaturated-phase temperature near interface is linear distribution, then

$$q_V = 2\lambda_{uns}(\nabla\alpha_{uns} \cdot \nabla T). \quad (20)$$

In the following, Eq. (19) is proved based on one-dimensional problem as shown in Fig. 1. $q_{V,i}$ can be obtained from Eq. (20).

$$q_{V,i} = 2\lambda_{uns}(\nabla\alpha_{uns,i} \cdot \nabla T_i) = 2\lambda_{uns} \left(\frac{\partial\alpha_{uns}}{\partial x} \right)_i \left(\frac{\partial T}{\partial x} \right)_i \quad (21)$$

where

$$\left(\frac{\partial\alpha_{uns}}{\partial x} \right)_i = \frac{\alpha_{uns,i+1} - \alpha_{uns,i-1}}{2\delta x} = -\frac{1}{2\delta x} \quad (22)$$

$$\left(\frac{\partial T}{\partial x} \right)_i = \frac{T_{i+1} - T_{i-1}}{2\delta x} = \frac{T_{sat} - T_{i-1}}{2\delta x} = \frac{1.5\delta x}{2\delta x} \cdot \frac{T_{sat} - T_{i-1}}{1.5\delta x} = \frac{3}{4} \frac{\partial T}{\partial n} \Big|_{uns} \quad (23)$$

Then Eq. (21) can be rewritten as

$$q_{V,i} = \frac{3}{4\delta x} \left(-\lambda_{uns} \frac{\partial T}{\partial n} \Big|_{uns} \right). \quad (24)$$

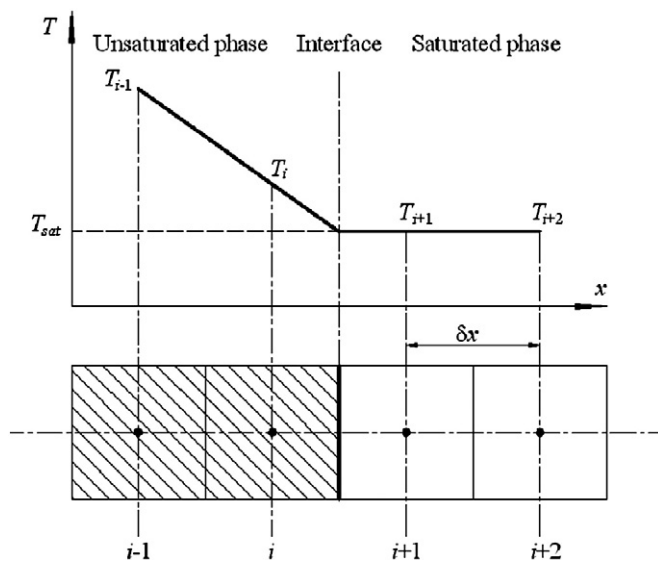


Fig. 1. Schematic diagram of interface, saturated phase, unsaturated phase and temperature distribution.

Similarly, $q_{V,i+1}$ can be written as

$$q_{V,i+1} = \frac{1}{4\delta x} \left(-\lambda_{uns} \frac{\partial T}{\partial n} \Big|_{uns} \right). \quad (25)$$

Substituting Eqs. (24) and (25) into the right side of Eq. (19), we can obtain

$$\int_{-l}^l q_V d\vec{l} = (q_{V,i}\delta x + q_{V,i+1}\delta x) \vec{n} = \left(-\lambda_{uns} \frac{\partial T}{\partial n} \Big|_{uns} \right) \vec{n} = \|\vec{q}_I\|. \quad (26)$$

Finally, the interfacial mass-transfer rate can be obtained based on Eq. (20):

$$\dot{m}_s = -\dot{m}_{uns} = \frac{q_V}{L} = \frac{2\lambda_{uns}(\nabla\alpha_{uns} \cdot \nabla T)}{L}. \quad (27)$$

4. Verification of phase change model

In this section, the phase change model is applied to solve one-dimensional Stefan problem and two-dimensional film boiling problem for verifying the accuracy of this model. Here, the fractional step method is used to treat the pressure-velocity coupling. The PLIC geo-reconstruct method [6] is applied to solve the volume fraction equation. The third-order MUSCL scheme [17] is adopted for the convective terms in momentum Eq. (8) and energy Eq. (13). A user defined code is developed to calculate the mass and energy transfer between both phases during the boiling and condensation process. This transfer is determined by the source terms \dot{m}_s , \dot{m}_{uns} and S_h in Eqs. (6), (7) and (13).

4.1. One-dimensional Stefan problem

The one-dimensional Stefan problem, as shown in Fig. 2(a), has served over and over again in CFD/NHT as a benchmark problem for testing the developed models [14,15,18]. In this problem, the vapor and liquid are considered incompressible and are initially in quiescent equilibrium. The wall temperature is higher than saturated temperature. The vapor near the wall experiences an increase in temperature and becomes superheated, which drives mass transfer at the interface. In this process, the vapor will always keep motionless while the liquid and the interface would be driven away from the wall.

The energy equation in the vapor phase can be written as

$$\frac{\partial T}{\partial t} = \frac{\lambda_v}{\rho_v C_{p,v}} \frac{\partial^2 T}{\partial x^2} \quad 0 \leq x \leq \delta(t) \quad (28)$$

where $\delta(t)$ is the interface position. The temperature boundary conditions are

$$T(x=0, t) = T_w \quad (29)$$

$$T(x=\delta(t), t) = T_{sat} \quad (30)$$

and the interfacial heat flux jump condition is

$$\rho_v v_l L = -\lambda_v \frac{\partial T}{\partial n} \Big|_{v,x=\delta(t)} \quad (31)$$

where v_l denotes the velocity at interfacial surface.

The exact interface position may be obtained by solving Eqs. (28)–(31) [19].

$$\delta(t) = 2\epsilon \sqrt{\frac{\lambda_v t}{\rho_v C_{p,v}}} \quad (32)$$

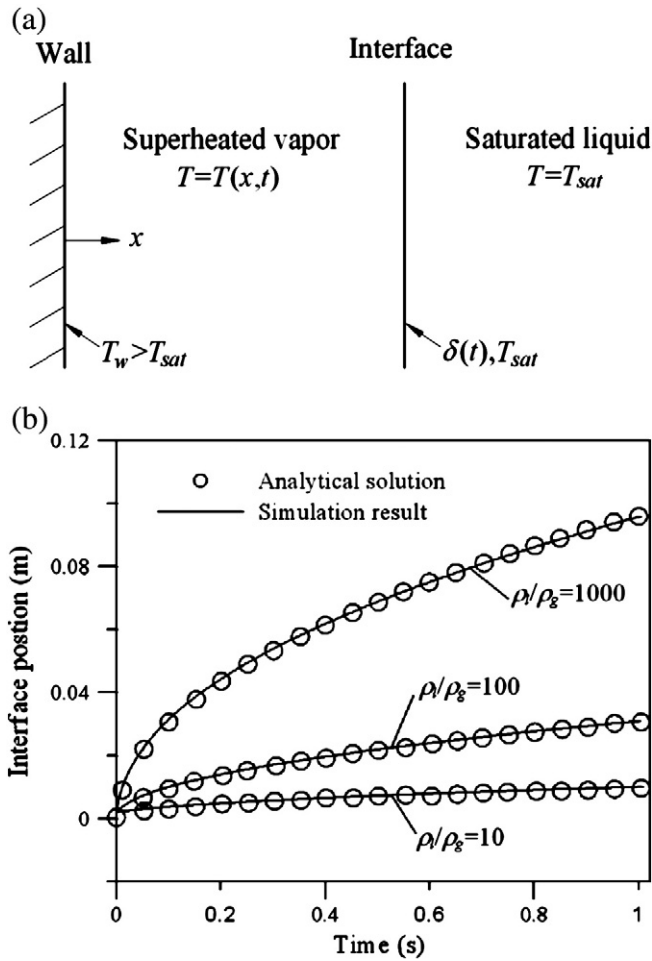


Fig. 2. (a) Schematic diagram and (b) interface positions with time for one-dimensional Stefan problem.

where ε is a solution to the transcendental equation

$$\varepsilon \exp(\varepsilon^2) \operatorname{erf}(\varepsilon) = \frac{C_{p,v}(T_w - T_{sat})}{L\sqrt{\pi}} \quad (33)$$

In this problem, the unsaturated phase is superheated vapor. Three different densities are considered $\rho_v = 0.001, 0.01$ and $0.1 \text{ kg}\cdot\text{m}^{-3}$. Thermal conductivity $\lambda_v = 0.005 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ and specific heat $C_{p,v} = 200 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$. The saturated phase is saturated liquid. Density $\rho_l = 1 \text{ kg}\cdot\text{m}^{-3}$. Based on our phase change model, we assume thermal conductivity $\lambda_l = 0 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ and specific heat $C_{p,l} = C_{p,v}$. Latent heat $L = 10000 \text{ J}\cdot\text{kg}^{-1}$. The difference between the wall and the saturated temperatures $\Delta T = T_w - T_{sat} = 10 \text{ K}$. The length of computation domain is 0.2 m . A uniform grid of 200 with a time step $1 \times 10^{-4} \text{ s}$ is used to solve the problem. Fig. 2(b) shows the interface positions with time at different density ratios. As shown in this figure, the simulation results agree very well with the exact analytical solutions, verifying the accuracy of this phase change model.

4.2. Two-dimensional film boiling problem

Fig. 3(a) shows the schematic diagram of two-dimensional boiling problem. The entire solid wall is covered by a layer of superheated vapor which is located below the saturated liquid. In this problem, the unsaturated phase is superheated vapor. $\rho_v = 5 \text{ kg}\cdot\text{m}^{-3}$, $\mu_v = 0.005 \text{ Pa}\cdot\text{s}$, $\lambda_v = 1 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$, $C_{p,v} = 200 \text{ J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$. The saturated

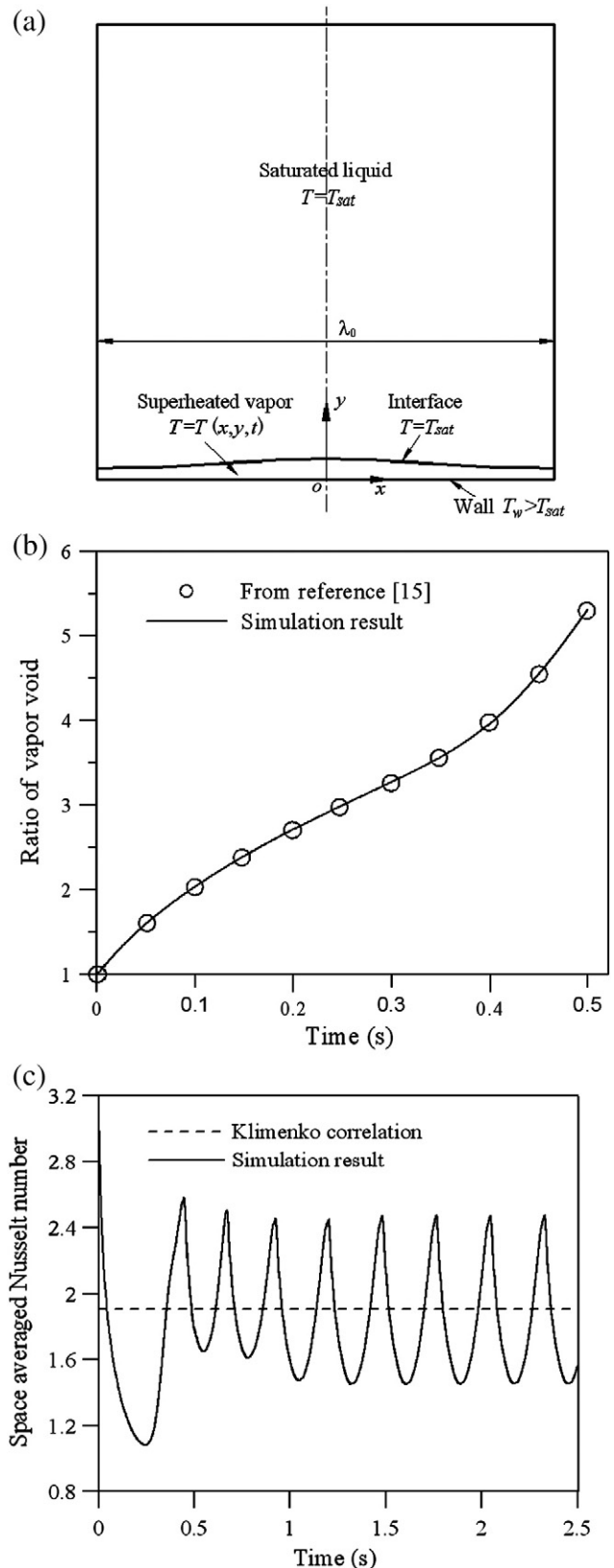


Fig. 3. (a) Schematic diagram, (b) ratios of vapor void to initial vapor void and (c) Nusselt number for two-dimensional film boiling problem.

phase is saturated liquid. $\rho_l = 200 \text{ kg}\cdot\text{m}^{-3}$, $\mu_l = 0.1 \text{ Pa}\cdot\text{s}$, $\lambda_l = 0 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ (assumed value), and $C_{p,l} = C_{p,v}$ (assumed value). Latent heat $L = 10000 \text{ J}\cdot\text{kg}^{-1}$, surface tension coefficient $\sigma =$

0.1 N·m⁻¹ and gravity acceleration $g=9.81 \text{ m}\cdot\text{s}^{-2}$. λ_0 shown in Fig. 3(a) is the unstable Taylor wavelength, which is expressed as

$$\lambda_0 = 2\pi \sqrt{\frac{3\sigma}{(\rho_l - \rho_g)g}} \quad (34)$$

Because of the symmetry of flow configuration, half of the region shown in Fig. 3(a) is selected as the computational region. The width and height of computational region are $\lambda_0/2$ and λ_0 , respectively. A uniform grid of 64(x) \times 128(y) with a time step 1×10^{-5} s is used to solve the problem. The velocity boundary condition at bottom wall is no-slip condition and the thermal boundary condition is fixed temperature 5 K higher than saturated temperature ($T_w = T_{sat} + 5$ K). The left and right vertical boundaries are considered symmetry boundaries and the top boundary is open with the pressure specified. We initialize the velocity to be zero, the liquid temperature to be saturated temperature and the vapor temperature to increase linearly for the interface to the wall. The initial interface position can be expressed as

$$y = \frac{\lambda_0}{128} \left(4.0 + \cos\left(\frac{2\pi x}{\lambda}\right) \right) \quad (35)$$

Fig. 3(b) shows the ratios of vapor void to initial vapor void in the formation process of initial bubble. As shown in Fig. 3(b), the results computed by our phase change model agree very well with those cited from reference [15], verifying the accuracy of our model.

Klimenko [20] analyzed the film boiling on horizontal plates based on some basic assumptions and obtained an expression for the Nusselt number.

$$Nu = \begin{cases} 0.19Gr^{1/3}Pr^{1/3}f_1 & \text{for } Gr \leq 4.03 \times 10^5 \\ 0.0216Gr^{1/2}Pr^{1/3}f_2 & \text{for } Gr > 4.03 \times 10^5 \end{cases} \quad (36)$$

where

$$f_1 = \begin{cases} 1 & \text{for } \beta \geq 0.71 \\ 0.89\beta^{-1/3} & \text{for } \beta < 0.71 \end{cases} \quad (37)$$

$$f_2 = \begin{cases} 1 & \text{for } \beta \geq 0.5 \\ 0.71\beta^{-1/2} & \text{for } \beta < 0.5 \end{cases} \quad (38)$$

In Eqs. (36)–(38), Gr , Pr and β are expressed as

$$Gr = \frac{\rho_v^2 g \lambda^3}{\mu_v^2} \left(\frac{\rho_l}{\rho_v} - 1 \right) \quad (39)$$

$$Pr = \frac{C_{p,v} \mu_v}{\lambda_v} \quad (40)$$

$$\beta = \frac{C_{p,v}(T_w - T_{sat})}{L} \quad (41)$$

λ is the characteristic length.

$$\lambda' = \sqrt{\frac{\sigma}{(\rho_l - \rho_v)g}} \quad (42)$$

In this problem, the Nusselt number calculated by Klimenko correlation (36) equals to 1.91.

In our simulations, the Nusselt number is computed as the dimensionless heat flux through the wall

$$Nu = \int_0^{\lambda_0/2} \left(\frac{\lambda'}{T_w - T_{sat}} \frac{\partial T}{\partial y} \Big|_{y=0} \right) dx \Big/ \frac{\lambda_0}{2} \quad (43)$$

Fig. 3(c) shows the Nusselt number calculated by our phase change mode. It changes periodically with time. The results are consistent with those presented in [15]. The time-averaged Nusselt number is 1.81, which has only a five-percent deviation with Klimenko correlation. All of these provide further evidence that our phase change mode is accurate.

5. Conclusion

In this paper, a vapor–liquid phase change model is proposed for the volume-of-fluid (VOF) method in FLUENT. This model is suitable for the case in which both unsaturated phase and saturated phase are present. It includes the following three part contents:

- (1) The unsaturated-phase thermal conductivity λ_{uns} and specific heat $C_{p,uns}$ are actual physical parameters.
- (2) The saturated-phase thermal conductivity λ_s and specific heat $C_{p,s}$ are assumed as zero and $C_{p,uns}$, respectively.
- (3) The interfacial mass-transfer rate $\dot{m}_s = -\dot{m}_{uns} = 2\lambda_{uns} (\nabla\alpha_{uns} \cdot \nabla T)/L$.

We verify our phase change model by one-dimensional Stefan problem and two-dimensional boiling problem. The results simulated by our model are found to be in excellent agreement with the analytical solutions or the calculation results by other authors. Because the model is high in accuracy and easy for operation in FLUENT, it is expected that the model will be promising in the computations of incompressible two-phase flow and heat transfer problems.

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