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A volume of fluid based method for vapor-liquid phase change simulation with numerical oscillation suppression

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ABSTRACT

A method of modeling phase change and suppressing numerical oscillation in vapor-liquid phase change simulation based on volume of fluid (VOF) is proposed in this study. The vapor-liquid interface is tracked by using VOF and reconstructed by applying a piecewise linear interface calculation (PLIC) scheme. Mass and heat transfer across the interface are modeled by employing a mass source term and an energy source term in the governing equations. In phase change model, the interface area needs to be calculated explicitly by assuming that the interface is linear in a cell. Expressions of two-dimensional interface length in the phase change model are also provided. The cause of the numerical oscillation, which may appear in the simulation, is analyzed. The analysis shows that small interfacial thermal resistance, large time step and ratio of interface area to cell volume are the causes of the numerical oscillation. An energy source donor-acceptor scheme is presented to suppress the numerical oscillation. One-dimensional Stefan problem, two-dimensional film boiling phenomenon and two-dimensional film condensation process were simulated using the model and scheme. Results validate the feasibility of using this method to simulate vapor-liquid flow with phase change. The numerical oscillations are also suppressed effectively in the simulations.

1. Introduction

Boiling and condensation can effectively transfer large amounts of heat because of the large amounts of energy in the form of latent heat. The two phase change processes are very important in extracting energy from various sources, such as solar, fossil, and nuclear fuels. Hydrodynamic and heat transfer processes in boiling and condensation are linked very closely. This coupling is much closer than that in single-phase flows [1]. In addition, it is extremely difficult to conduct accurate and effective experimental measurements because the spatial scales are small and the time constants are rapid in the phase change process. The importance and complexity have led to decades of experimental and theoretical studies. Substantial experimental and analytical studies in the past have resulted in numerous empirical relations or correlations associated with phase change. Workers have successfully matched experimental data to the relations or correlations. However, empirical finding or correlation is only applicable to the specific conditions under which it was developed. Most of these findings or correlations cannot be applied to new situations because of their limited range of applicability. Numerical methods for predicting phase change problems have become popular and reliable as a result of the rapid development of computer hardware and numerical algorithms [2]. Accurate numerical simulations can reveal details of heat and mass transfer processes that are not measurable in experiments. Such procedures will facilitate understanding of underlying physical behavior.

Two main difficulties exist in accurate phase change simulations. One difficulty is the accurate tracking of vapor-liquid interfaces in phase change problems. Different interface tracking methods have been used to simulate the phase change problems. Son and Dhir [3] used a coordinate transformation technique supplemented by a numerical grid generation method to construct a grid system aligned with the interface. This method was used to simulate saturated film boiling on a horizontal surface. The same method was also applied by Banerjee and Dhir [4] in studying subcooled film boiling. Welch [5] used an interface tracking method in conjunction with a finite volume method on a moving unstructured mesh to simulate the axisymmetric vapor bubble growth. When the interface changes, these methods require remeshing to be adapted to the interface deformation. Thus, these methods show a limited applicability because of their inability to cope with large interfacial distortion or change in topology. This limitation was later overcome by Juric and Tryggvason [6]. They used front track-

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Nomenclature

A_i	interface area in a cell (m^2)
c_p	specific heat [J/(kg K)]
E	energy per unit mass (J/kg)
$\vec{F}_{CSF}$	surface tension induced volume force (N/m^3)
$\vec{g}$	gravity acceleration vector (m/s^2)
Ga	Galileo number
h_{fg}	latent heat (J/kg)
k	phase change mass transfer coefficient [kg/(m^2 s K)]
l_{cr}	critical wavelength (m)
l_m	most unstable wavelength (m)
$\dot{m}$	mass flux across the interface [kg/(m^2 s)]
$\vec{n}$	unit normal vector
Nu	Nusselt number
p	pressure (Pa)
Pr	Prandtl number
q	heat flux (W/m^2)
Q_E	produced heat per second (W)
r	mass transfer intensity factor (s^{-1})
S_E	energy source term (W/m^3)
S_m	mass source term [kg/(m^3 s)]
t	time (s)
Δt	time step (s)
T	temperature (K)
$\vec{u}$	velocity vector (m/s)
V_c	volume of a cell (m^3)
x, y	Cartesian coordinates

Greek symbols

α	volume fraction
δx	cell width (m)
δ	thickness (m)
λ	thermal conductivity [W/(m K)]
σ	surface tension (N/m)
κ	surface curvature
ρ	density (kg/m^3)
μ	dynamic viscosity (Pa s)
ν_v	kinematic viscosity (m^2/s)

Subscripts and superscripts

a	acceptor
c	condensing
d	donor
e	evaporating
i	interface
l	liquid
max	maximum
min	minimum
sat	saturation
v	vapor
w	wall

ing method, which is based on finite difference method, to simulate boiling flow. A fixed grid was used in the method. A separate front marked the interface, and was only modified near the front to make a grid line follow the interface. This method was also used by Esmaeeli and Tryggvason [7] to simulate three-dimensional film boiling. A level set method can also overcome this limitation. The interface in the level-set method is captured and tracked by the level-set function, which is defined as a signed distance from the interface [8]. This method was used by Son and Dhir to simulated axisymmetric film boiling flows [8] and the bubble merger process on a single nucleation site during pool nucleate boiling [9]. Mukherjee and Dhir [10] used this method to simulate the lateral merger of vapor bubbles during nucleate pool boiling. Luo et al. [11] combined the variable density projection method with level-set method to simulate immiscible interfacial flows with phase change. Wu et al. [12] simulated subcooled nucleate boiling coupling level-set method with a moving-mesh method. Despite its extensive application, level-set method is found to have a deficiency in preserving volume conservation [13]. Volume of Fluid (VOF) method is another method that can model the vapor-liquid interface and it does not have the deficiency in preserving volume conservation. Volume fraction is employed in VOF to track the interface. Various technologies for simulating phase change problems have been used in VOF to obtain an accurate curvature and to smoothen the discontinuous physical quantities near the interfaces, for example, the PLIC scheme [13–22], the modified high resolution interface capturing (HRIC) scheme [23,24], and the conservative interpolation scheme for interface tracking (CISIT) [25]. The PLIC scheme is one of the most popular methods used in the applications.

The other important difficulty is the need to model the mass and heat transfer of phase change at the interface. The mass and heat flux across the interface needs first to be modeled. Two approaches were commonly used to obtain the interfacial mass flux in the existing references. One approach involves direct or indirect application of energy jump condition at the interface [5,7–13,15,17,19,20,22,25,26]. The condition can be expressed as

$$\dot{m}_v h_{fg} = -\dot{m}_l h_{fg} = q = \left[\left(-\lambda_l \frac{\partial T}{\partial n}\Big|_l\right) - \left(-\lambda_v \frac{\partial T}{\partial n}\Big|_v\right)\right] \cdot \vec{n}, \tag{1}$$

where $\vec{n}$ is a unit vector normal to the interface and pointing toward the vapor. In Eq. (1), $q > 0$ means evaporation and $q < 0$ means condensation. However, this method does not consider the interfacial thermal resistance for phase change. The other approach is based on the interfacial thermal resistance model proposed by Schrage [21,27–31]. In the model, the mass flux at the interface can be determined by

$$\dot{m}_v = -\dot{m}_l = \frac{2\beta}{2-\beta}\sqrt{\frac{M}{2\pi R}}\frac{\rho_v h_{fg}(T - T_{sat})}{T_{sat}^{3/2}}, \tag{2}$$

where coefficient β represents the fraction of molecules transferred from one phase to the other during phase change.

Then, volumetric source terms should be derived from the flux model to apply it to the phase change simulations. Two commonly methods are available by which the source terms can be constructed in the references. The first method is using the feature of the volume faction [31]. The feature can be expressed as

$$\int_\Omega |\nabla\alpha| d\Omega = \int_S dS, \tag{3}$$

where α can be either the liquid or vapor volume fraction. Thus, the integration represents the interface area in theory. After using this feature, the mass source terms in the first method can be written as [8,19,20,28,30,31]:

$$\begin{cases} S_{m,v} = \dot{m}_v |\nabla\alpha| \\ S_{m,l} = -\dot{m}_v |\nabla\alpha| \end{cases}. \tag{4}$$