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Numerical modeling of three-phase flow with phase change using the level-set method

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ABSTRACT

This article presents a numerical model for three-phase flow with phase change. Two level-set functions are defined to capture the two interfaces involved in the problem, i.e. the interface between two fluids and the interface between the fluid with its phase change component. With these two level-set functions, all the interfaces can be treated within the same numerical framework. Numerical solution is performed on a fixed mesh using the finite volume method. Surface tension effect is treated using the continuum surface force model. The model is validated against one- and two-dimensional vaporization problems. Finally, the model is demonstrated for different three-phase flow with phase change problems involving (1) a liquid with a rising condensing vapor bubble and a falling immiscible liquid droplet and (2) solidification in stratified two-fluid flow with a growing solid layer.

1. Introduction

Flow with phase change is widely encountered in many engineering applications. Examples include, but are not limited to, flow boiling in heat exchangers [1], quenching of hot plates [2], laser induced melting in 3D printing process [3] and crystal growth [4]. In all of these systems, a certain amount of material changes its physical form, e.g. solid vs. liquid (melting or solidification) and liquid vs. gas (vaporization or condensation). Generally, there is a distinct interface separating the two different phases. Such interface evolves over time. In additional to mass transfer across the interface, phase change usually involves a large amount of heat absorbed or released at the interface. Therefore, the interface dynamics is intimately coupled to heat and mass transfers in a phase change process.

Numerous experimental and numerical modeling efforts are performed on studying of phase change process to further understand the underlying physics. Numerical modeling of such problem is complex. The principal difficulty lies in the fact that phase change is a "moving boundary problem" with "jump" conditions across the interface. Generally, large difference in thermal properties is encountered across the interface, e.g. water-steam system with density and viscosity of water: 958 $\mathrm{kg/m^3}$ and 2.82×10^{-4} Pa·s vs. steam: 0.598 $\mathrm{kg/m^3}$ and 1.23×10^{-5} Pa·s. Numerically, mass, momentum and energy jump conditions need special treatments. Moreover, depending on the level of modeling, different numerical methods consider the phase change interface as a "sharp front" or a "mushy zone" with apparent thickness. The temperature at the interface is also a question although it is frequently assumed to be maintained at saturation temperature depending on pressure [5]. Nevertheless, extensive numerical work still attempts to address different issues encountered in the phase change process. Significant progress has been made in the past few decades. A representative review for pool boiling study can be found in the work of Dhir et al. [6].

Central to the numerical simulation of phase change problem is the movement of the phase change interface. Given the way the interface is handled, current numerical methods for predicting the interface movement can be categorized into two categories, i.e. front tracking method and front capturing method. In the front tracking method, the interface is tracked explicitly while in the front capturing method, the interface is captured implicitly through an indicator function. Most of the existing works for two-phase flow with phase change is based on either one of these two techniques.

Welch [7,8] is among the first to employ moving mesh method to track the phase change interface. He adopted unstructured moving mesh near the interface in the simulation of vapor bubble

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Nomenclature

a	constant
A	constant (m/s)
b	source term
c_p	specific heat (J/kg·K)
d	distance (m)
$\vec{g}$	gravity (m^2/s)
h	latent heat (J/kg)
H	height of domain (m)
$H(\phi)$	smoothed heaviside function
k	thermal conductivity (W/m·K)
K	constant
L	length of domain (m)
$\dot{m}$	mass flux ($kg/m^2 \cdot s$)
$\hat{n}$	unit normal at the interface
p	pressure (Pa)
R	radius (m)
S	area (m^2)
$S(\phi)$	Sign function
t	time (s)
$\hat{t}$	unit tangent to the interface
T	temperature (°C)
$\vec{u}$	velocity vector (m/s)
x, y	Cartesian coordinate

Greek symbols

α	constant (m^3/kg)
δ	thickness of vapor region (m)
$\delta(\phi)$	Dirac delta function
Γ	interface
θ	dimensionless temperature
ϕ	level set function (m)
φ	component of $\vec{u}_{i,ext}$
ε	interface thickness (m)
μ	dynamic viscosity (kg/m·s)
ρ	density (kg/m^3)
σ	surface tension (N/m)
κ	curvature (1/m)
Ω	domain of interest

Subscripts

i	interface
i,ext	extension velocity
m	$11'$ or 12
nb	neighborhood of calculated point
P	point in calculation
sat	saturation
w	wall
1	fluid 1 region
$1'$	fluid $1'$ region
2	fluid 2 region
o	initial state

growth. Remeshing is required each time step so that the mesh always coincides with the interface. Therefore, Welch's approach [7,8] is limited to the cases where the interface does not distort significantly. Juric and Tryggvason [5] developed a front-tracking method which is called "single-field formulation" to model film boiling. The method to certain extent alleviates the limitation in Welch's approach [7,8] of having interface with small deformation. This method is extended further by Esmaeeli and Tryggvason [9,10] by improving its numerical technique. It is applied to model film boiling for both single vapor bubble and multiple vapor bubbles. Vu et al. [11] developed a numerical model for solidification around a circular cylinder under forced convection using the front-tracking/finite difference method. Generally, front tracking methods are still difficult to cope with interface undergoing large deformations or even topological changes. In order to overcome such difficulties, the volume-of-fluid (VOF) method [12] and the level-set method [13] based on the front capturing methods are widely used. VOF method is adopted by Welch and Wilson [14], Hardt and Wondra [15], Kunkelmann and Stephan [16] and Magnini et al. [17], to name a few, for modeling of phase change problems in different applications. One of the challenges for employing the VOF method is the required interface reconstructions during the calculation procedure. Son [18] has developed a numerical model for phase change problem based on level-set method. Soon after, the model is then adopted by many researchers to study different phase change problems [19–23].

For more general problems, three-phase flow with phase change can also occur in engineering applications. Examples are enhanced oil recovery via steam injection involving steam, water and oil [24], casting involving solid alloy, molten alloy and air [25] and latent heat thermal energy storage utilizing phase-change materials (PCM) involving solid PCM, liquid PCM and air [26]. For these flows, there are multiple unknown evolving interfaces, e.g. in a steam-water–oil system, there exist steam-water, steam-oil and water–oil interfaces. Accurate modeling requires these interfaces to be either tracked and captured. Due to the complex nature of the coupled mass, momentum and energy transports between the three phases at these interfaces, numerical modeling of three-phase flow with phase change is relatively limited in existing literatures if compared to the counterparts of two-phase flow with phase change.

Kim et al. [27] investigated freezing of water partially filled in an annulus with an upper air layer. There are three phases involved, i.e. ice, water and air. The moving interfaces are tracked using a moving mesh method with appropriate coordinate transformations to represent the interfaces. Assis et al. [28] and Solomon et al. [29] presented a model to study the melting process of PCM in spherical shell with an upper air layer. The liquid PCM-air interface is captured using the VOF method. However, the liquid–solid PCM interface is determined using the enthalpy-porosity approach [30]. The front-tracking/finite difference method was used for modeling of drop solidification on a cold plate [31] and solidification of liquid PCM in an open (air) horizontal circular cylinder [32]. In these works [27–32], there is a solid phase. Therefore, only two remaining phases can flow.

However, for three-phase flow with phase change involving liquid, its vapor and another immiscible liquid, all phases flow. Besides, surface tension effect needs to be accounted for at all interfaces. A model for film boiling in liquid jet impingement on a high-temperature plate was developed by [33]. The conservation equations for the three phases: liquid, vapor, and air, are solved with phase change liquid–vapor interface captured using the sharp-interface level-set formulation and liquid–air interface represented using a step function. Lee et al. [34] employed the model of Kim and Son [33] to investigate quenching of a hot plate in a liquid jet impingement involving liquid, vapor and air. Conjugate heat transfer with the hot plate included was incorporated.

The above two categories of three-phase flow with phase change, i.e. with one phase undergoes either solidification/melting or condensation/vaporization, can be treated within a unified for-