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Discretization and implementation of a sharp interface model for interfacial heat and mass transfer during bubble growth

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ABSTRACT

Simulations of phase change rely on methods to compute heat and mass transfer at the interface. Current methods estimate the mass transfer with interpolation functions or by assuming a local temperature difference between saturation and interface. This work reports a method that uses a single cell around the interface to find the interfacial temperature gradient, and a linear interpolation normal to the interface to find the temperature of the mixture cell (cell with an interface). The one-cell algorithm for sharp interface and mass transfer (OCASIMAT) simplifies the estimation of the mass transfer and mixture cell temperature and improves accuracy. The proposed approach leads to a more realistic representation of the heat and mass transfer at the interface with a sharp discontinuity on the thermal properties at the interface and with mass transfer only at the cells with an interface. Simulations of planar interface evaporation and spherical bubble growth demonstrate the application of the proposed approach. Results indicate that OCASIMAT accurately predicts the temperature distributions near the interface and the interface displacements.

1. Introduction

Applications of evaporation and boiling are found in heat sinks for electronics cooling, nuclear and fossil fuel powered steam generators, distillation columns, concentrated solar power systems, glass melting furnaces, desalination chambers, and heat and mass exchangers. In order to increase the performance and safety margins of these applications, there is a need to develop tools that predict the localized interfacial dynamics during the phase change process. The analysis of bubble growth has been addressed by computer simulations, which employ methods for mass transfer and for the dynamic interfacial interaction. Accurate methods available in the technical literature to simulate bubble growth require advanced algorithms that present significant challenges in the analysis of phase change at the interface level. Other approaches require simplifying assumptions at the expense of accuracy. A new approach is presented in this paper to simplify the interfacial mass transfer computations and to include a sharp interface representation while preserving accuracy.

Simulations of boiling and evaporation have computed the mass transfer with the local difference between the saturation and an interface temperature [1–9]. This approach requires an iterative procedure to match the new interface position with the corresponding interface temperature [10]. Similarly, Strotos et al. adopted [11] an evaporation model that considered a difference between the saturation and bulk pressures in the simulation of droplet evaporation. Maki and Kumar [12] simulated droplet evaporation by assuming a temperature difference between the interface and a saturation temperature in addition to a pressure difference. These models avoid the identification of the interface location since they use local differences instead of gradients at the interface. However, the models depend on an empirically derived accommodation coefficient, and therefore provide only an indirect estimation of the mass transfer.

Other phase change simulations estimate the mass transfer with the temperature gradients at the center or faces of the surrounding cells rather than at the interface [13–16]. Haelssig et al. [13] computed the temperature gradient at the center of the mixture cell (a cell with an interface). The temperature gradient considered the temperature of the neighboring cells (cells around the mixture cell) and the normal vector. Sun et al. [14] computed the temperature gradient at the faces of the mixture cell. These approaches ignore the interface location for the purpose of easy calculation, but they sacrifice accuracy by computing the temperature gradient at a certain distance from the interface. Moreover, interpolation functions are needed to find proper temperatures of

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Nomenclature

A_i	interface surface area (m^2)
D	distance interface to cell center (m)
C	large coefficient
C	specific heat (J/kg K)
F	volume-fraction
h_{fg}	latent heat (J/kg)
K	thermal conductivity (W/m K)
K	curvature (1/m)
m''	mass flux (kg/s m^2)
$\hat{n}$	unit normal vector
p	pressure (N/m^2)
r	radial coordinate (r)
R	bubble radius (m)
S_M	momentum source term (N/m^3)
S_T	energy source term (K/s)
sd	distance interface to cell center (m)
T	temperature (K)
t	time (s)
V_c	cell Volume (m^3)
v	velocity (m/s)
X	interface position (m)
x	x-position (m)
α	thermal diffusivity (m^2/s)
β	bubble growth constant
μ	dynamic viscosity (Pa-s)
ξ	growth rate constant
ρ	density (kg/m^3)
σ	surface tension (N/m)
ϕ	density ratio

Subscripts

l	liquid
sat	saturation
v	vapor

the mixture cells or the neighboring cells that lie on the opposite side of the interface.

Another approach is to compute the mass transfer with temperature gradients at the interface [17–21]. Akthar and Kleis [17,18] defined the temperature gradient with the distance from the neighboring cell center to the interface along the Cartesian directions. Schlottke and Weigand [21] adopted a similar approach to simulate droplet evaporation. Their mass transfer model considered vapor mass fractions at the interface and neighboring cells rather than temperatures. When the interface does not intersect with the centerlines of the mixture cells, the method is no longer applicable, and the gradient could be found with an interpolated mixture cell temperature [15]. Kunkelmann and Stephan [19] computed the mass transfer with an interface temperature, the saturation temperature, and the distance from the interface to the mixture cell. The main difficulty with this method is the estimation of the interface temperature, which requires an iterative procedure.

The present work provides a one-cell algorithm for sharp interface and mass transfer (OCASIMAT) that simplifies the estimation of mass transfer and improves accuracy. The proposed approach finds the temperature gradient at the interface with the temperature of only one computational cell without interpolation functions. To account for a sharp interface, a mathematical expression directly estimates the temperature of the mixture cells based on the temperature gradient at the interface. Two fundamental problems involving interfacial heat and mass transfer are used to evaluate and validate this approach; these problems include planar interface evaporation and spherical bubble growth.

2. Numerical model

This section is divided into two subsections. Section 2.1 shows the governing equations for the interface tracking and the mass transfer. It also shows the equations for momentum and energy transport. Section 2.2 focuses on the temperature gradients at the interface and on the temperature of the cells with an interface.

2.1. Governing equations

The volume-of fluid (VOF) equation Eq. (1) for the vapor volume-fraction tracks the interface.

$$\frac{\partial}{\partial t}(F_v) + \nabla \cdot (F_v \overrightarrow{v_v}) = \frac{m''}{\rho_v}\frac{A_i}{V_c} \tag{1}$$

where F_v is the vapor volume fraction on each cell, ρ_v is the vapor density, $\overrightarrow{v_v}$ is the vapor velocity, m'' is the mass flux, A_i is the interface surface area, and V_c is the cell volume. Eq. (2) is a constraint for the liquid volume fraction, F_l, at each cell.

$$F_l + F_v = 1 \tag{2}$$

The piecewise-linear scheme reconstructs the interface, which assumes the interface shape in each cell as a straight line. The interface inclination and the volume-fraction on each cell find the interface surface area A_i. Eq. (3) estimates the mass flux at each mixture cell:

$$m'' = \frac{k_l \nabla T_i}{h_{fg}} \tag{3}$$

where k_l is the liquid thermal conductivity, h_{fg} is the latent heat of evaporation, and ∇T_i is the temperature gradient at the interface. The main challenge in Eq. (3) is the estimation of the temperature gradient at the interface. The interfacial temperature gradient requires a temperature reconstruction algorithm. The present work proposes a method to find the temperature gradient at the interface with a single liquid cell. The proposed approach (explained in Section 2.4) is easy to implement and improves the accuracy of the mass transfer estimation.

The momentum conservation equation Eq. (4) finds the pressure and the velocity on the liquid and vapor phases:

$$\rho\left[\frac{\partial \vec{v}}{\partial t} + (\nabla \cdot \vec{v})\vec{v}\right] = -\nabla p + \nabla \cdot \mu \nabla \vec{v} + \nabla \cdot \mu \nabla \vec{v}^{T} + S_M \tag{4}$$

where p is the pressure, μ is the viscosity, and S_M accounts for the surface tension effects. The continuous surface force (CSF) model proposed by Brackbill et al. [22] accounts for surface tension effects. Eq. (5) estimates the surface tension volume force:

$$S_M = \sigma \frac{\rho k \nabla F_v}{0.5(\rho_v + \rho_l)} \tag{5}$$

where σ is the surface tension. The interface curvature, k, is estimated as:

$$k = \nabla \cdot \hat{n} \tag{6}$$