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A sharp-interface phase change model for a mass-conservative interface tracking method

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ABSTRACT

A new phase-change model has been developed for a mass-conservative interface tracking method. The mass transfer rate is directly calculated from the heat flux at the liquid–vapor interface, and the phase change takes place only in the cells which include this interface. As a consequence of the sharpness of the mass transfer rate distribution, the velocity jump across the interface can be captured, and high accuracy can be maintained. The method has been implemented in an incompressible Navier–Stokes equations solver employing a projection method based on a staggered finite-volume algorithm on Cartesian grids. The model has been verified for one-dimensional phase-change problems and a three-dimensional simulation of a growing vapor bubble in a superheated liquid under zero gravity condition. The computed results agree with theoretical solutions, and the accuracy of the model is confirmed to be of second-order in space using a grid refinement study. A three-dimensional simulation of a rising vapor bubble in a superheated liquid under gravity has been performed as a validation case, and good agreement with experimental data is obtained for the bubble growth rate. As a demonstration of the applicability of the method to engineering problems, a nucleate boiling simulation is presented with a comparison to experimental data. Good agreement is obtained for the bubble shapes and the bubble departure period. In all the simulation cases, strict mass conservation is satisfied.

1. Introduction

Nucleate boiling heat transfer is one of the most efficient modes of heat transfer under high heat-flux conditions, and is used in many technical applications, such as refrigeration, cooling systems, boilers, heat exchangers, etc. Although there are many applications, the evaluation of boiling heat transfer still relies on empirical methods, because numerical simulation methods are not sufficiently well established. The long-term goal of our research is to formulate a phase-change model within the framework of Computational Fluid Dynamics (CFD) to predict boiling heat transfer. In this paper, we propose a mass-conservative phase-change model which can be applied for the simulation of nucleate boiling heat transfer.

The first attempt to simulate boiling using a CFD technique is attributed to Welch [1]. A two-dimensional, moving, triangular grid system was used to represent the liquid–vapor interface, but the method was limited to two-dimensional computations without topology change of the interface shape. In order to simulate large deformation of the liquid–vapor interface, an interface tracking methods were introduced to phase-change simulations in the late 1990s. A Level Set (LS) method was introduced by Son and Dhir [2], a Front Tracking (FT) method by Juric and Tryggvason [3], and a Volume Of Fluid (VOF) method by Welch and Wilson [4]. In these studies, two-dimensional film boiling simulations were undertaken.

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The phase-change model coupled with LS [2] has been continuously improved, mainly due to the efforts of Dhir's group [5], and applied to nucleate boiling situations [6], bubble merge processes during nucleate boiling [7,8], film boiling from a horizontal cylinder [9,10], nucleate boiling with high heat fluxes [11], and sub-cooled pool boiling [12]. In these simulations, phase-change phenomena can be simulated under various conditions using a contact-angle treatment [6], a micro-region model [6], or an Immersed Boundary Method (IBM) to represent the solid surfaces [9]. However, the drawback of the phase-change model coupled with LS is that the conservation is not guaranteed, because LS is a non-conservative approach [13]. In addition to Dhir's group, Gibou et al. [14] have developed a phase-change model based on LS using a "ghost-fluid" method, and two-dimensional film boiling has been simulated. Tanguy et al. [15] also use LS-based phase change model with ghost fluid method, and computed an evaporating water droplet in air. Can and Prosperetti [16] have also used an LS-based phase change model to investigate vapor bubble dynamics under the assumption that the velocity and temperature fields in the vapor are negligible. Recently, Houim and Kuo [17] have developed a phase-change model based on LS and a ghost-fluid method for compressible reacting flows. A two-dimensional Riemann problem is defined and solved for the coupled system of interface, vapor and liquid droplet.

In the phase-change model coupled with FT [3], the liquid–vapor interface is explicitly represented by surface segments. Esmaeeli and Tryggvason [18,19] have studied three-dimensional film boiling from multiple horizontal cylinders using IBM [20]. Although Tryggvason and his co-workers were able to demonstrate the usefulness of the method in film boiling simulations, implementation of the FT algorithm is far from straightforward, especially in regard to the topology changes at the liquid–vapor interfaces.

In the phase-change model coupled with VOF [4], the mass transfer rate is calculated directly from the heat flux at the liquid–vapor interface. Hereafter, we refer to the model as VOF-DHF (Direct Heat Flux). Using VOF-DHF, Welch and Rachidi [21] simulated a two-dimensional film boiling with the conjugate heat transfer, and Agarwal et al. [22] computed unsteady, periodic bubble release during film boiling in two dimensions. Ghosh et al. [23,24] applied VOF-DHF in spherically symmetric geometry to compute spherical bubble growth. Yuan et al. [25] extended VOF-DHF to a body-fitted coordinate system to compute film boiling from a horizontal cylinder, while Haelssig et al. [26] simulated two-dimensional countercurrent flow with phase change. However, in these studies, VOF-DHF is restricted to two-dimensional coordinate system or spherically symmetric geometry, and has not been applied to three-dimensional situations such as a spherical bubble growth problem, which is suitable for a verification of a phase change model. One of the main reasons for this is difficulty in discretization; a spherical bubble cannot be kept spherical during the growth due to the numerical error in phase change model. Akhtar and Kleis [27] conducted three-dimensional bubble growth simulation using VOF-DHF with local grid refinement, but the computed result shows the deformed bubble shape. Very recently, Ma and Bothe [28] have proposed a VOF-based evaporation model including the Marangoni effect. Using two separate temperature fields, the authors show that the interfacial heat transfer may be calculated very accurately.

Meanwhile, Hardt and Wondra [29] have developed a phase-change model based on VOF in which the mass transfer rate is estimated from the evaporation heat transfer coefficient proposed by Schrage [30]. In order to avoid deformation of the liquid–vapor interface, which is the main problem in using the VOF-DHF approach, the mass transfer rate is artificially smeared over 4–5 computational cells surrounding the interface, and then the distribution of the mass transfer rate is again artificially shifted to the liquid side for condensation, and to the vapor side for boiling. This shifting is considered to cause errors in the flow velocity, pressure and temperature distributions, because the phase change does not occur at the liquid–vapor interface itself, but in the liquid or vapor phase, as appropriate. However, one merit of the model is the ease of implementation, and so features in as appropriate implemented into commercial CFD software such as ANSYS Fluent® or OpenFOAM®. Kunkelmann and Stephan [31,32] simulated spherical bubble growth and three-dimensional nucleate boiling implementing the Hardt model [29] in OpenFOAM®.

Tomar et al. [33] have proposed a phase change model based on CLSVOF – a Coupled LS and VOF approach. The method is reported to both conserve mass and capture complicated interface topologies accurately, but only two-dimensional computations have so far been presented, and without validation cases. Jamet et al. [34] have developed a second-gradient approach to phase-change simulation based on thermodynamics. The method has been applied only in a one-dimensional phase-change situation, and its extension to two or three dimensions are postponed to future works. Badillo [35] has developed a quantitative phase-field model, also based on thermodynamics. Bubble growth simulations have been performed assuming spherical symmetry and compared with an analytical solution and measured data. However, phase-field computations in three dimensions have not yet been reported.

To the authors' knowledge, there appears not to exist a three-dimensional, mass-conservative phase change model for which the mass transfer rate is calculated directly from the heat flux at the interface. In this paper, we propose such a model. The mass transfer rate is directly computed from the heat flux at the liquid–vapor interface, in the same way as with the VOF-DHF approach, but with full dimensional capability. The phase change takes place only in the cells containing the liquid–vapor interface, with the velocity jump across the interface captured sharply. The model is formulated in Cartesian geometry, and verified by means of one-dimensional problems and three-dimensional simulation of a vapor bubble growth in superheated liquid under zero gravity condition. As a validation case, a three-dimensional simulation of a rising vapor bubble in a superheated liquid under gravity is performed, and the bubble growth rate is compared with experiments. As a demonstration of the applicability of the method to engineering problems, a nucleate boiling simulation is presented, and the results are compared with experiments.