Numerical modeling of thermocapillary two-phase flows with evaporation using a two-scalar approach for heat transfer

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ARTICLE INFO

ABSTRACT

A one-field model is derived from the sharp interface continuum mechanical balances for two-phase evaporative and thermocapillary flows. Emphasis is put on a clear distinction of the different velocities at the interface which appear due to phase transfer. The one-field model is solved numerically within a Finite Volume scheme and the interface is captured using an extended Volume of Fluid method, where the interface is reconstructed linearly with the PLIC technique. The numerical heat transfer is based on a two-scalar approach where two separate temperature fields are used for the temperature inside the two phases. This results in an accurate treatment of the interfacial heat transfer, specifically the interface temperature which is crucial numerically, both for evaporation and thermocapillarity. The method is validated for two-phase heat conduction, with analytical solution in case of no evaporation and with experimental measurement in case of incorporated evaporation effect. The method is applied to realistic cases dealing with non-uniformly heated thin liquid films, i.e. liquid films on (i) structured heated substrates and (ii) locally heated substrates. The numerical predictions in terms of flow pattern, surface deformation, temperature and velocity are compared with experiments conducted at the Université Libre de Bruxelles for (i) and at the Technische Universität Darmstadt for (ii). Qualitative agreement is achieved and shows the potential of this approach to simulate thermocapillary flows with dynamically deformable interfaces combined with evaporation.

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1. Introduction

Thermocapillary flows occur in multi-phase systems due to temperature-dependent surface tension. Such flows play an important role in various industrial applications in which the key processes like heat and mass transfer take place at a fluid interface, such as in material processing, cooling technology, painting, drying etc. The reason for the surface tension to be inhomogeneous along the interface can be mainly found in its dependence on temperature or on concentration of adsorbed surface active agents, e.g. [20,7,9]; for numerical modeling of the influence of surfactants see also [2] and the references given there. The resulting local surface tension gradients will cause tangential motion of the fluid interface which will generate flows in the ambient bulk phases due to viscous stress. This effect is called Marangoni effect or Marangoni convection. In inhomogeneously heated thin liquid films, which can be widely found in cooling technologies, the thermal Marangoni effect has a dominant influence on the fluid dynamics of the system. The resulting surface tension-driven convection can enhance

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heat transfer, or cause film rupture which will lead to a local heat crisis [41,40]. Furthermore, evaporation and its influence on the local temperature due to latent heat is a significant factor interacting with the Marangoni effect. For quantitative prediction of such processes a numerical model by means of Direct Numerical Simulation (DNS) is desired. Based on the previous work by [22], which builds on an extended Volume of Fluid (VOF) method to simulate the thermally driven Marangoni effect, where the surface tension only depends on temperature, the present work aims to further improve and extend the previously developed numerical method in order to apply it to the above mentioned practically relevant phenomena in which evaporation is to be considered.

The DNS of evaporation without thermocapillary effect has been considered by several authors. Juric and Tryggvason [15] use a front tracking method for boiling flows. Jung and Sato [14] perform DNS of a high Schmidt number flow over a droplet in 3D. They employ a moving, unstructured mesh consisting of prisms at the interface to resolve the viscous boundary layer and tetrahedral cells in the remaining domain. Tanguy et al. [35] present a level set approach and utilize the Ghost Fluid Method [10] to enable the use of high order discretization schemes at the interface. By developing a model to calculate the interface velocities considering the volume change due to evaporation, they are able to cover the physical effects related to the Stefan flow. The calculations have been done in 2D and have not yet been validated against experimental data or correlations from the literature. Gibuo et al. [12] present a similar method based on level set and Ghost Fluid, as well. They preserve the discontinuity of all variables except the viscosity which is smoothed across the interface. The method is applied to simulate film boiling in 2D. Son and Dhir [33] developed a model for boiling flow based on the level set approach. Chen et al. [6] incorporate evaporation in a VOF-based simulation of gas bubbles moving in a bounded viscous liquid. Their phase change model captures the volume change in the fluids due to mass transfer at the interface. The different velocites at the interface are not taken into account in the model. A method using the VOF approach for boiling flow was presented by [37], who applied their method to 2D film boiling. Davidson and Rudman [8] present a VOF-based algorithm for the calculation of transport processes across deforming interfaces, using the analogy between heat and mass transfer. The algorithm is described assuming planar or axisymmetric flows and does not consider volume changes due to phase change. The calculation of heat transfer is separated for the two phases with respect to the enthalpy as transported quantity, while the temperature is treated as a single field based on an average in the interface cells. Nikolopoulos et al. [25] investigate the behavior of liquid droplets impinging onto a hot substrate using the VOF-method and adaptive mesh refinement. They are able to predict the levitation of the drops above the Leidenfrost temperature and to calculate parameters of the splashing process below the Leidenfrost point. Schlottke and Weigand [31] use the VOF method to simulate deformed evaporating droplets in high Reynolds number flows and can predict the global Sherwood number under droplet surface deformation. [18] developed a VOF-based model with adaptive mesh refinement for nucleate boiling, where a level-set extension is employed to reconstruct the sharp interface for a more accurate computation of the evaporation rate. Simulations of single bubble growth and detachment as well as lateral merger of two bubbles using this model show good agreement with experiments. Strotos et al. [34] apply the VOF-method without the numerical reconstruction of the interface but with a local grid refinement technique to simulate multi-component droplet evaporation under forced convection in a hot environment. The model is validated with respect to evaporating time and droplet temperature.

As already pointed out in [22], for quantitative prediction of thermocapillary flows the common VOF approach, based on a one-field formulation of the two-phase model, does not deliver the necessary accuracy of the interfacial heat transfer which is especially crucial for thermocapillary flows. Out of the motivation of enhancing the interfacial heat transfer computation, the present paper first derives a rigorous one-field numerical modeling of evaporative two-phase flows suitable for numerical solution using interface capturing methods. On this basis, and building on experience with handling interfacial discontinuities in VOF-based DNS of mass transfer [3] as well as with the method involving sharp temperature fields due to [30], we present a two-scalar ghost-fluid like approach as a powerful tool for numerical modeling of evaporative thermocapillary flows.

This paper is organized as follows. In Section 2, we recall the mathematical model in sufficient generality to include evaporation and the different velocities at the interface. In Section 4, after the main elements of the general numerical scheme are introduced, special focus is put on the development of the two-scalar approach. This is followed by some numerical tests in Section 5. In Section 6, two applications on thermocapillary flows in liquid films are introduced which are investigated numerically and some qualitative results are given. Finally, several conclusions are drawn in Section 7.

2. Mathematical formulation

We consider incompressible two-phase flows of immiscible Newtonian fluids with heat transfer and phase change. The mathematical model applied in this work is based on continuum mechanics and employs a sharp interface of zero thickness, where the deformable and moving interface $\Sigma(t)$ between the two phases is assumed to have zero mass. The resulting two-phase model contains two sets of equations for the two phases and certain jump conditions at the interface. This model is not in a convenient form for numerical solution which is intended in a finite volume context. Therefore, we derive a one-field formulation of the two-phase model, where the whole domain is governed by only one set of equations. This is done by means of volume averaging where the equations are not written locally, but for control volumes containing spatially averaged quantities.