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Buoyancy-thermocapillary convection of volatile fluids under atmospheric conditions

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ABSTRACT

Convection in a layer of fluid with a free surface due to a combination of thermocapillary stresses and buoyancy is one of the classic problems of fluid mechanics. Although extensively studied, it is still not fully understood. In particular, neither the effect of phase change nor the thermal boundary conditions at the liquid–vapor interface have been properly described. These two intimately related issues have a significant impact on the stability of the flow and transitions between different convective patterns. The objective of this paper is to develop and validate a comprehensive numerical model which properly describes both heat transfer and phase change at the liquid–vapor interface, as well as the transport of heat and vapor in the gas layer, which is ignored by the vast majority of theoretical studies with minimal justification. We present a numerical investigation of convection in a long cell filled with a volatile fluid and air, and investigate the changes in convective patterns due to with changes in the applied horizontal temperature gradient. We also explore how variations in the wetting properties of the fluid and lateral confinement (three-dimensionality) affect the flow. While the numerical results have been found to be in general agreement with existing experimental observations, we have also discovered an unexpected phenomenon: a region of evaporation near the cold wall and a region of condensation near the hot wall.

1. Introduction

The flow patterns and dynamic behaviors of liquid films driven by thermocapillarity have attracted the attention of researchers for many years. Initially the interest was driven by applications to crystal growth in microgravity environments, with the focus on liquid metals and, correspondingly, low values of the Prandtl number Pr (typically $Pr < 0.05$). Smith and Davis [1,2] were the first to perform a linear stability analysis of thermocapillary (or Marangoni) convection in a laterally unbounded liquid layer subject to a horizontal temperature gradient. Ignoring buoyancy effects, they predicted that the return-flow basic state would undergo an instability towards either surface waves (for $Pr < 0.15$) or hydrothermal waves (for $Pr > 0.15$) above a critical Marangoni number Ma, which characterizes the magnitude of thermocapillary stresses. In particular, hydrothermal waves were predicted to travel in the direction of the thermal gradient. Their predictions have since been thoroughly tested and verified both in microgravity and for thin films in terrestrial conditions. A thorough overview of these experiments is presented in a review paper by Schatz and Neitzel [3].

More recently the motivation for further studies of this problem has shifted rather dramatically due to the increased demands on the performance of various cooling technologies. Thermal management is a major issue for a wide range of applications. Many of the modern cooling technologies exploit the large latent heats associated with phase change at the free surface of volatile liquids, allowing compact devices to handle very high heat fluxes. The basic geometry of such cooling devices is similar to the problem investigated under microgravity – a liquid film on the walls of a sealed cavity, under its own vapor as well as noncondensable gases, such as air. Heating one end of the cavity, and cooling the other, establishes a horizontal temperature gradient that drives the flow. However, in addition to thermocapillarity, under terrestrial conditions one often has to consider body forces such as gravity and hence buoyancy. The relative importance of buoyancy and thermocapillarity is quantified by the ratio of Rayleigh and Marangoni numbers $Bo = Ra/Ma$, referred to as the dynamic Bond number.

The first systematic study of buoyancy-thermocapillary convection was performed by Villers and Platten [4] who studied convection in acetone ($Pr = 4.24$) experimentally and numerically using a

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one-sided model that ignored heat and mass transfer in the gas phase. For low *Ma* they found the same featureless return flow that characterizes pure thermocapillary convection. However, as *Ma* was increased, they discovered that the convective patterns which emerge when $Bo = O(1)$ differ substantially from the case dominated by thermocapillarity ($Bo \ll 1$). Instead of hydrothermal waves, they found a steady flow featuring multiple convection rolls. These rolls were found to rotate in the same direction, unlike the case of pure buoyant (or Rayleigh–Bénard) convection. Moreover, unlike the hydrothermal waves which form at an angle to the direction of the thermal gradient, the steady multicellular state features rolls that align in the transverse direction. At even higher *Ma* the steady state was found to be replaced by an oscillatory multicellular pattern that was also unlike a hydrothermal wave. The convection rolls were observed to travel in the direction opposite to hydrothermal waves.

Similar results were obtained later by De Saedeleer et al. [5] for decane ($Pr = 15$) and Garcimartin et al. [6] for decane and 0.65 cSt and 2.0 cSt silicone oil ($Pr = 10$ and 30, respectively) in cavities with strong confinement in the spanwise direction. Riley and Neitzel [7] performed one of the most extensive and detailed experimental studies of convection in a 1 cSt silicone oil with $Pr = 13.9$ in a rectangular cavity with a spanwise dimension comparable to the streamwise dimension. They discovered that a direct transitions from steady, unicellular flow to hydrothermal waves takes place for small values of the dynamic Bond number ($Bo \lesssim 0.2$), while for $Bo \gtrsim 0.2$ the results are similar to those of Refs. [4–6]: first a transition to steady co-rotating multicells, and upon further increase in *Ma*, to an oscillatory multicellular pattern. Riley and Neitzel also determined the critical values of *Ma* and the wavelength λ of the convective pattern as a function of *Bo*.

The linear stability analysis of Smith and David [1] provides an accurate description of experimentally observed convective patterns for low *Bo*. However, it fails to predict the patterns that emerge for $Bo = O(1)$, although the spatially uniform return flow at low *Ma* is found to be consistent [7] with the analytical solution for the velocity and temperature [8,9] away from the lateral boundaries. The majority of the studies that have performed linear stability analysis around this analytical solution ignore the effect of the end walls and, hence, predict incorrect patterns. In particular, for adiabatic boundary conditions at the top and bottom of the liquid layer, Parmentier et al. [10] predict transition to traveling waves rather than steady multicellular pattern for $Pr \leqslant 7$ fluids regardless of the value of *Bo*. Chan and Chen [32], who used similar assumptions, also predict transition to traveling waves for a $Pr = 13.9$ fluid. Moreover their critical *Ma* and wavelength λ do not match the experiment [7]. In both cases the traveling waves are oblique for smaller *Bo* and become transverse for $Bo > Bo_c = O(1)$.

Mercier and Normand [11] showed that transition to a stationary convective pattern can take place if the adiabatic boundary conditions are replaced with Newton's cooling law, although that requires an unrealistically large surface Biot number ($Bi \gtrsim 185/Bo$). Moreover, the predicted pattern corresponds to longitudinal convection rolls, while in the experiments [4–7] transverse rolls were observed. In a subsequent paper Mercier and Normand [12] considered the effects of the end walls, which they described as spatial disturbances superimposed on the uniform base flow. It was found that depending upon the Prandtl number, recirculation rolls would develop near the hot end ($Pr > 4$), near the cold end ($Pr < 0.01$) or at both end walls ($0.01 < Pr < 4$).

Priede and Gerbeth [13] where the first to consider the effect of the end walls on the stability of the base flow. They used a generalized linear stability analysis to argue that hydrothermal waves correspond to a global oscillatory instability which dominates at lower *Bo*, while the stationary patterns result from a local absolute instability which, for higher *Bo*, has a lower threshold value of *Ma* than the global oscillatory instability. Their prediction agrees remarkably well with the threshold values found by Riley and Neitzel [7].

Understanding the convective patterns above the threshold of the primary instability requires a numerical approach. To date, the majority of numerical studies (e.g., Villers and Platten [4], Ben Hadid and Roux [14], Mundrane and Zebib [15], Lu and Zhuang [16], Shevtsova et al. [17]) have focused on 2D flows. Furthermore, just like the linear stability analyses, existing numerical studies assume that the temperature gradient is generated by imposing fixed temperatures on the two end walls; the free surface is flat and non-deformable; the thermal boundary conditions on the bottom wall and the interface are either adiabatic or conducting; and phase change is negligible. Unlike the other studies, Ji et al. [18] consider the effect of phase change on the thermal boundary condition at the free surface, but they ignore buoyancy.

While the 2D approximation may be appropriate in describing some experiments, the validity of the rest of these assumptions is questionable. Validating them is one of the main objectives of the present study. Furthermore, while the numerical simulations reproduce some features of the experimental studies [4–7], they fail partially or completely in describing other features, most notably the structure of the boundary layers near the end walls which defines both the temperature gradient in the bulk and controls the dynamics of oscillatory states at higher *Ma*. Description of these boundary layers requires a detailed model of transport of heat (and mass) in both the liquid and the vapor layer, as well as phase change at their interface.

We present such a model of two-phase flow and its numerical implementation in the following Section. The results obtained using this model in a specific test problem, namely buoyancy-thermocapillary convection in a sealed rectangular cavity where the dimension along the temperature gradient is much greater than the other two dimensions and any evaporation must be balanced by condensation are presented and discussed in Section 3 and our conclusions – in Section 4.

2. Mathematical model

2.1. Governing equations

Existing analytical and numerical studies of buoyancy-thermocapillary convection, with rare exceptions, use one-sided models where heat and mass transport in the gas phase are incorporated indirectly through boundary conditions at the liquid–vapor interface. While such an approach might be justifiable for nonvolatile liquids since air is a relatively poor conductor of heat, volatile liquids require a two-sided model. For volatile liquids, phase change can lead to significant heat fluxes in the liquid layer due to the latent heat released or absorbed at the interface. The interfacial mass flux (which defines the heat flux) cannot be computed reliably without a proper model of bulk mass transport in the gas phase.

Two-sided models have been formulated previously by Wang et al. [19] for a meniscus in a microtube, by Pan and Wang [20] for a meniscus in an exposed pore, and by Wang et al. [21] for an open groove. These models, however, assume rather than compute the shape of the free surface and do not account for the advective transport of heat and mass in the gas phase.

In order to describe convection in both volatile and nonvolatile fluids, the heat and mass transport in both phases must be modeled explicitly. Both the liquid and the gas phases can be considered incompressible, since the fluid velocities $\mathbf{u}$ are much smaller than the speed of sound at small length scales. Hence the continuity equation reduces to $\nabla \cdot \mathbf{u} = 0$. Because the fluid velocities can, however, be large enough for inertial effects to be significant, the