



Buoyancy-thermocapillary convection of volatile fluids under their vapors



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ABSTRACT

Convection in a layer of fluid with a free surface due to a combination of thermocapillary stresses and buoyancy has been studied extensively under atmospheric conditions. However, recent experimental results have shown that removing most of the air from a sealed cavity significantly alters the flow structure and, in particular, suppresses transitions between different convection patterns found at atmospheric conditions. On the other hand, removing air has a very small effect on the flow speed, while a simple analytical estimate predicts that complete removal of noncondensable gases such as air should reduce the flow speed by an order of magnitude. To understand these unexpected results, we have formulated and numerically implemented a detailed transport model that takes into account mass and heat transport in both phases in the absence of noncondensables. The model was used to investigate how the flow is affected by the magnitude of the (poorly defined) accommodation coefficient and by the temperature jump across the liquid-vapor interface predicted by some phase change models. Our results eliminate both effects as possible explanations for the unexpected experimental observations, suggesting that the small amount of air left in the cavity in the experiments is the most likely, albeit somewhat unexpected, explanation for the observations.

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1. Introduction

Convection in liquid films driven by horizontal temperature gradients has attracted attention in the past due to applications to crystal growth in microgravity environments, where evaporation is negligible, buoyancy plays no role, and the flow is driven by thermocapillarity. More recently, the focus shifted to flows driven by a combined action of capillary pressure, thermocapillary forces, and buoyancy with phase change playing an increasingly important role due to applications in thermal management in terrestrial environments. In particular, devices such as heat pipes and heat spreaders, which use phase change to enhance thermal transport, are typically sealed, with noncondensables (such as air), which can impede phase change, removed [1].

The liquid film is almost always in contact with a mixture of its own vapor and air. The fundamental studies on which the design of such devices is based, however, often do not distinguish between different compositions of the gas phase. The experimental studies

are typically performed in geometries that are not sealed and hence contain air at atmospheric pressure, while most theoretical studies ignore phase change completely. Those that do consider phase change use transport models of the gas phase that are too crude to properly describe the effect of noncondensables on the flow in the liquid layer. Yet, as a recent experimental study by Li et al. [2] shows, noncondensables play an important and nontrivial role, so the results in one limit cannot be simply extrapolated to the other.

We have introduced a proper two-sided model for volatile fluids which provides a detailed description of heat and mass transport in both the liquid and the gas phase dominated by noncondensables in a separate paper [3]. This model, as well as previous experimental studies of volatile and nonvolatile fluids by Villers and Platten [4], De Saedeleer et al. [5], Garcimartin et al. [6], Riley and Neitzel [7] and Li et al. [2], shows that volatile and nonvolatile fluids have similar behavior at atmospheric conditions. At dynamic Bond numbers of order unity, the flow in the liquid layer is relatively fast and transitions from a steady unicellular pattern (featuring one big convection roll) to a steady multicellular pattern (featuring multiple steady convection rolls) to an oscillatory pattern (featuring multiple unsteady convection rolls) as the applied temperature

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gradient is increased. Numerical studies of nonvolatile fluids by Villers and Platten [4], Ben Hadid and Roux [8], Mundrane and Zebib [9], Lu and Zhuang [10], and Shevtsova et al. [11] come to the same basic conclusion, justifying the use of one-sided models in the limit where the gas phase is dominated by noncondensables.

Here our focus is on the opposite limit, where the gas phase is dominated by vapors rather than noncondensables. As the experiments of Li et al. [2] conducted for a volatile silicone oil at dynamic Bond numbers $Bo_D \approx 1$ demonstrate, transitions between different convection patterns are suppressed under vapor, and the flow structure remains the same (i.e., qualitatively similar to the unicellular flow under air) when the magnitude of the applied temperature gradient is varied. Moreover, in the vapor-dominated limit, the flow speeds were found to be comparable to those in the air-dominated limit, although existing transport models predict that the flow speeds in the absence of noncondensables should decrease substantially.

Proper interpretation of these experimental observation requires fundamental understanding of two-phase flows in confined geometries in the (near) absence of noncondensables, which is currently lacking. There are very few theoretical studies of this limit. Zhang et al. [12] performed an analytical investigation of a model of a sealed rectangular heat-pipe with pure vapor (no air) above an essentially flat liquid layer. Their model, however, was based on a large number of assumptions (Stokes flow, negligible buoyancy, negligible advective fluxes, infinite evaporation and Marangoni numbers) that do not hold for the experimental studies [2]. Kuznetsov and Sitnikov [13] and Kaya and Goldak [14] proposed and numerically investigated models of heat pipes which do not include buoyancy or Marangoni effects, do not conserve mass, and treat the liquid phase in a very restrictive way (as Darcy or lubrication flow). Kafel and Turan [15] and Fadhl et al. [16] proposed and investigated crude models of thermosyphons which treat the fluid as a mixture of the liquid and vapor phase, with phase change occurring in the bulk rather than at a (non-existing) interface.

To address this deficit, we introduce a comprehensive two-sided model of two-phase flow of a volatile fluid in confined and sealed geometries due to an applied temperature gradient in the absence of noncondensables. This model is described in detail in Section 2. Results of the numerical investigations of this model are presented, analyzed, and compared with experimental findings in Section 3. Finally, Section 4 presents our conclusions.

2. Mathematical model

2.1. Governing equations

The vast majority of theoretical studies of buoyancy-thermo-capillary convection is based on one-sided models where heat and mass transport in the gas phase are not solved for directly, but rather are incorporated indirectly through boundary conditions at the liquid-vapor interface. As we have shown using a two-sided model [3] which describes heat and mass transport in both phases, Newton's law of cooling, which is the basis of most one-sided models, is generally invalid for convection at atmospheric conditions. Hence, there is no reason, *a priori*, to believe that it should hold in the absence of noncondensables. In order to describe convection in volatile fluids in the absence of noncondensables, the heat and mass transport in both phases must be modeled explicitly.

Zhang et al. [12] have previously formulated a two-sided model for the problem considered here in the limit of vanishing Reynolds number and infinite Marangoni and evaporation numbers [17] and obtained an analytical solution for the case of a pinned contact line

and an essentially flat interface. Unfortunately, almost none of these assumptions actually hold in the experiments of Li et al. [2], requiring development of a general two-sided model that does not rely on any of these assumptions. Such a model, based on the one described in Ref. [3] is presented below.

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 momentum transport in the bulk should be described by the Navier–Stokes equation

$$\rho(\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho(T)\mathbf{g} \quad (1)$$

where p and T are the fluid pressure and temperature, ρ and μ are the fluid's density and viscosity, respectively, and \mathbf{g} is the gravitational acceleration.

Following standard practice, we use the Boussinesq approximation, retaining the temperature dependence only in the last term to represent the buoyancy force. This is consistent with the assumption of incompressibility, since the relative change in the density due to temperature variation is usually quite small: less than 10% for the vapor and less than 4% for the liquid in the examples considered below. (To verify the validity of this approximation, we also performed the simulations with temperature dependence included for all material parameters and found only minor differences in the results.) Specifically, in the liquid phase

$$\rho_l = \rho_l^* [1 - \beta_l (T - T^*)], \quad (2)$$

where ρ_l^* is the reference density at the reference temperature T^* and $\beta_l = -(\partial \rho_l / \partial T) / \rho_l$ is the coefficient of thermal expansion. Here and below, subscripts l , v and i denote properties of the liquid and vapor phase, and the liquid-vapor interface, respectively. For the vapor, which is assumed to be an ideal gas,

$$\rho_v = p_v / \bar{R}_v T, \quad (3)$$

where $\bar{R}_v = R/M_v$, R is the universal gas constant, and M_v is the molar mass.

The total mass of fluid in a sealed geometry is conserved,

$$\int_{\text{liquid}} \rho_l dV + \int_{\text{gas}} \rho_v dV = m_t, \quad (4)$$

where m_t is the total mass of the working fluid in both phases. The densities of liquid and vapor are related to the temperature and pressure through (2) and (3). Furthermore, the solution of the Navier–Stokes equation defines the pressure field p up to a constant p_o , so that absolute pressure is

$$p_v = p + p_o, \quad (5)$$

where the pressure offset p_o can be computed from (4):

$$p_o = \left[\int_{\text{gas}} \frac{1}{\bar{R}_v T} dV \right]^{-1} \left[m_t - \int_{\text{liquid}} \rho_l dV - \int_{\text{gas}} \frac{p}{\bar{R}_v T} dV \right]. \quad (6)$$

Finally, the transport of heat is described using an advection-diffusion equation

$$\partial_t T + \mathbf{u} \cdot \nabla T = \alpha \nabla^2 T, \quad (7)$$

where $\alpha = k/\rho C_p$ is the thermal diffusivity, k is the thermal conductivity, and C_p is the heat capacity, of the fluid. The inclusion of advection terms in both transport equations can be justified by computing the Reynolds and thermal Peclet numbers, presented below in Table 5.

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