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The effect of noncondensables on buoyancy-thermocapillary convection of volatile fluids in confined geometries



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ABSTRACT

Recent experimental studies have shown that buoyancy-thermocapillary convection in a layer of volatile liquid subjected to a horizontal temperature gradient is strongly affected by the presence of noncondensable gases, such as air. Specifically, it was found that removing most of the air from a sealed cavity containing the liquid and its vapors significantly alters the flow structure and, in particular, suppresses transitions between the different convection patterns found at atmospheric conditions. Yet, at the same time, the concentration of noncondensables has almost no effect on the flow speeds in the liquid layer, at least for the parameter range studied in the experiments. To understand these results, we have formulated and numerically implemented a detailed model that accounts for mass and heat transport in both phases as well as the phase change at the interface. The predictions of this model, which assumes that the gas phase is dominated by either noncondensables have a large effect on the flow at concentrations even as low as 1%, i.e., values much lower than those achieved in experiment.

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1. Introduction

Convection in volatile fluids with a free surface due to a combination of thermocapillary stresses and buoyancy has been studied extensively due to applications in thermal management. In particular, devices such as thermosyphons, heat pipes, and heat spreaders, which use phase change to enhance thermal transport, are typically sealed, with most of the noncondensables (such as air), which can impede phase change, removed [1]. However, air tends to dissolve in liquids and be adsorbed into solids, so removing it completely is usually not feasible. Hence, the liquid film almost always remains in contact with a mixture of its own vapor and some 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 (e.g., varying amounts of air in the system). The vast majority of experimental studies was performed in geometries that are not sealed and hence contain air at atmospheric pressure. Yet, as a recent experimental study of convection in a volatile silicone oil (hexamethyldisiloxane) by Li et al. [2] showed, noncondensables can play an important role, so the results in one limit cannot be simply extrapolated to the other. Theoretical studies, on the other hand, tend to use a piecemeal approach based on breaking up the entire system into an "evaporator," a "condenser," and an "adiabatic region" in-between [3,4], often without checking whether such partitioning is justified or attempting to correlate the transport processes in the three regions.

The effect of noncondensables on filmwise condensation of vapors in simple geometries (thin liquid layers of condensate on flat or cylindrical surfaces) is reasonably well understood. In particular, in the absence of noncondensables, the heat transfer coefficient is controlled by the thickness of the draining film [5]. Condensation is reduced dramatically in the presence of noncondensables. In this case thermal resistance is typically dominated by the diffusion of vapors through a layer of noncondensables that accumulate next to the condensate film, which can be described using boundary layer theory for both free convection [6] and forced convection [7]. For instance, very small amounts of noncondensation rate, and the corresponding heat transfer coefficient, for steam condensation [6].

The vast majority of theoretical studies of buoyancy-thermoca pillary convection use one-sided models which describe transport

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in the liquid, but not the gas phase and ignore phase change, with both phase change and transport in the gas phase indirectly incorporated through boundary conditions at the liquid-vapor interface [8–12]. The predictions of such models are mostly consistent with experimental studies of volatile and nonvolatile fluids at ambient (atmospheric) conditions [8,13–15,2] which find that, for dynamic Bond number of order unity, the flow in the liquid layer transitions from a steady unicellular pattern (featuring a single large 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 gradient (and hence the Marangoni number) is increased.

Indeed, at atmospheric conditions phase change is strongly suppressed due to diffusion of vapors through air, so phase change plays a relatively minor role. However, upon closer examination, one finds that one-sided models fail to predict some important features of the problem. We have recently introduced a comprehensive two-sided model [16–18] of buoyancy-thermocapillary convection in confined fluids which provides a detailed description of momentum, heat and mass transport in both the liquid and the gas phase as well as phase change at the interface *in the entire system*. This model shows that at atmospheric conditions Newton's Law of Cooling, which serves as a foundation for all the one-sided models, completely breaks down [18]. Furthermore, one finds, rather counter-intuitively, that there are regions of evaporation (condensation) next to the cold (hot) end wall of the cavity containing the fluid [17].

In comparison, very few studies have been performed in the (near) absence of noncondensables. One notable exception is the study of Li et al. [2], who performed experiments for a volatile silicone oil. They found that the transitions between different convection patterns were suppressed when the concentration of noncondensables was reduced. In particular, only the steady unicellular regime is observed over the entire range of imposed temperature gradients at the lowest average air concentration investigated (14%). Interestingly, the experiments also show that, at small imposed temperature gradients, the flow structure and speeds remain essentially the same as the air concentration decreases from 96% (ambient conditions) to 14%, which corresponds to a reduction by more than two orders of magnitude in the partial pressure of air.

There are at present no theoretical models that are capable of explaining these experimental observations. The theoretical studies [19–23] available to date employ extremely restrictive assumptions and/or use a very crude description of one of the two phases. Our own two-sided model [18], which treats the gas phase as pure vapor, correctly predicts the suppression of transitions between convection patterns. However, it also predicts that thermocapillary stresses essentially vanish and the flow speed decreases substantially, which is not consistent with experimental observations. The high flow velocities found in experiment imply that thermocapillary stresses remain significant, which suggests that the presence of noncondensables in the gas phase, even at rather low concentrations, has a profound effect on the flow and has to be accounted for.

Hence, to better understand the effect of noncondensables on heat and mass transport in volatile fluids in confined and sealed geometries, our two-sided model [16–18] was further generalized to describe situations where the gas phase is dominated by vapor, but still contains a small amount of noncondensables [24]. The model is described in detail in Section 2. The results of the numerical investigations of this model are presented, analyzed, and compared with experimental observations in Section 3 and our summary and conclusions are presented in Section 4.

2. Mathematical model

2.1. Governing equations

We describe transport in both the liquid and the gas phase using a generalization of the pure-vapor model [18]. The present model is very similar to the one introduced in Ref. [17] (which describes transport at atmospheric conditions when the gas phase is a binary mixture dominated by air), but now the gas phase is dominated by vapor, rather than air. Both phases are considered incompressible and the momentum transport in the bulk is described by the Navier–Stokes equation

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

where *p* is the fluid pressure, ρ and μ are the fluid's density and viscosity, respectively, c_a is the concentration of air, and **g** is the gravitational acceleration. (The air is noncondensable, so $c_a = 0$ in the liquid phase.) Following standard practice, we use the Boussinesq approximation, retaining the temperature and composition dependence only in the last term to represent the buoyancy force. In the liquid phase

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

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, g, v, a, and i denote properties of the liquid and gas phase, vapor and air component, and the liquid–vapor interface, respectively. In the gas phase

$$\rho_g = \rho_a + \rho_v, \tag{3}$$

where both vapor (n = v) and air (n = a) are considered to be ideal gases

$$p_n = \rho_n \overline{R}_n T, \tag{4}$$

 $\overline{R}_n = R/M_n, R$ is the universal gas constant, and M_n is the molar mass. The total gas pressure is the sum of partial pressures

$$p_g = p_a + p_v. \tag{5}$$

On the left-hand-side of (1) the density is considered constant for each phase. We set it equal to the spatial average of $\rho(T, c_a)$.

To ensure local mass conservation of air, which is the less abundant component in the gas phase, we describe mass transport using the advection–diffusion equation for its density

$$\partial_t \rho_a + \mathbf{u} \cdot \nabla \rho_a = D \nabla^2 \rho_a, \tag{6}$$

where *D* is the binary diffusion coefficient of one component in the other. For a volatile fluid in confined geometry, the external temperature gradient causes both evaporation and condensation, with the net mass of the fluid being globally conserved

$$\int_{\text{liquid}} \rho_l dV + \int_{\text{gas}} \rho_v dV = m_{l+v},\tag{7}$$

where $m_{l+\nu}$ is the total mass of liquid and vapor. The total pressure in the gas phase is $p_g = p + p_o$, where the (constant) pressure offset p_o is

$$p_{o} = \left[\int_{\text{gas}} \frac{dV}{\overline{R}_{\nu}T} \right]^{-1} \left[m_{l+\nu} - \int_{\text{liquid}} \rho_{l} dV - \int_{\text{gas}} \frac{p dV}{\overline{R}_{\nu}T} \right].$$
(8)

The concentrations (or, more precisely, the molar fractions) of the two components can be computed from the equation of state using the partial pressures

$$c_n = p_n/p_g. \tag{9}$$

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