

Phase field models for Marangoni convection in planar layers

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A collection of methods is presented for describing Marangoni convection in two-layer systems in the phase field formalism. The models consist of the Navier-Stokes equation with an extra term of phase field, the heat equation, and a spatiotemporal evolution equation for the phase field. In this theoretical description the fluid-fluid interface becomes diffuse and free of interface conditions. 2D convective patterns are shown for incompressible, compressible, and compressible evaporating fluids.

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1. Introduction

The study of simplified models is an important part of the search for more general and systematic theories of complex systems with multi-interfaces. The phase field models treat thermodynamically multi-phase systems with complicate and involved time-dependent interface geometries by tackling the problem continuously, inclusive of the interfacial region. This continuous variation is realized with an additional phase field which contains information about the local state of the system composition. With the help of this field one can continuously express – from one medium to the other – all the system parameters: density ρ , viscosities η , λ , heat capacity c , thermal conductivity κ . In this way the basic equations are written only once for the whole system and the explicit interface conditions are eliminated. Proposed for the first time by Langer in an ad hoc manner, the phase field methodology has recently achieved considerable importance in modeling solidification phenomena [1-3] and crystal growths [4,5]. In fluid media the diffuse interface model was used for studying the spreading of thin liquid layers on a solid surface [6] or the phase separation near the liquid-gas critical point [7]. We extend this model to another problem with material interface: the Marangoni convection induced by thermo-capillary effect in immiscible liquid-gas systems with external heating. 2D numerical simulations will be reported for incompressible, compressible, and compressible evaporating fluids far from criticality.

2. Model

For immiscible liquid-gas superposed layers the most natural phase field function is the density (scaled here to the liquid density), assumed to be $\rho=1$ for the liquid phase and $\rho=0$ for the gas phase. We introduce the contribution of the phase field in the classical form of

Navier-Stokes equation by minimizing the free-energy functional for the equilibrium state. The Helmholtz free-energy functional is given by:

$$F = \int_V \left[f_0(\rho) + \frac{K(T)}{2} (\nabla\rho)^2 \right] dV, \quad (1)$$

with $f_0(\rho)$ the free-energy density of an homogeneous fluid far from interface. For $f_0(\rho)$ a continuous function of density is required with two symmetrical minima: one corresponding to $\rho=1$, for the bulk in the liquid state, and another one to $\rho=0$, namely for the bulk in the gas phase. We choose $f_0(\rho)$ in the following form:

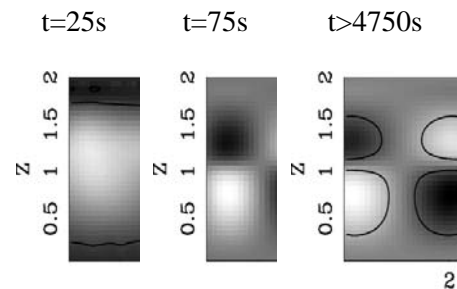


Fig. 1. Time series for the stream-function in the surface-tension-driven instability. The plots follow from the model 1 and correspond to a silicon-oil-air system heated from below. The contour lines in the third panel mark the reaching of the saturation state.

$$f_0(\rho) = C\rho^2(1-\rho)^2 / 2 \quad (2)$$

To describe situations in the presence of interfaces the free-energy functional is generalized by including gradient contributions to the total internal energy. The second term

in (1) describes the interfacial energy and contributes to the free-energy excess of the interfacial region which defines the surface tension coefficient [8]:

$$\sigma = \int_{-\infty}^{+\infty} K \left(\frac{\partial \rho_0}{\partial z} \right)^2 dz \quad (3)$$

(ρ_0 denotes the density profile in the stationary state). Surface tension effects are incorporated into the model through a modified stress tensor in the Navier-Stokes equations. So, applying the Lagrangian formalism for minimizing the free-energy functional (1) one finds out in Navier-Stokes equation a supplementary term of phase-field. This supplementary term represents – in the frame of phase-field formalism – the substitute of classical interfacial conditions for the stress balance (for more details see [9]):

$$\rho \frac{d\vec{v}}{dt} = -\nabla p + \rho \nabla (\nabla \cdot (K \nabla \rho)) + \nabla \cdot (\eta \nabla \vec{v}) + \nabla (\lambda \nabla \cdot \vec{v}). \quad (4)$$

The pressure term p is connected to the free-energy density via the thermodynamic relation: $p = \rho \partial f / \partial \rho - f$. We intend to describe with our model the Marangoni convection driven by the surface tension gradient (so-called thermo-capillary effect). In this aim we have to assume K as a function of the temperature $K = K - K_T T$, ($K_T > 0$, $K_T \ll K_0$). Thus, the theoretical description has to be completed by the heat equation for the temperature field and by the continuity equation for the density.

3. Simulations

Model 1: incompressible fluids with rigid interface.

The most simple model assumes both fluids being incompressible which implies: $\nabla \cdot \vec{v} = 0$. In this case we introduce the stream function $\psi(x, z)$ in place of the velocity field $\vec{v}(x, z)$: $\vec{v} = (\partial \psi / \partial z) \vec{i} - (\partial \psi / \partial x) \vec{k}$, fact which will essentially simplify the analytical and the numerical computations. For the stationary motionless state, the Navier-Stokes equation (4) with the symmetrical “double-well” potential given by the relation (2) admits the analytical solution:

$$\rho_0(z) = 1 / [1 + \exp((z-1)/\ell)] \quad \ell \propto \sqrt{K/C}. \quad (5)$$

For small enough values of ℓ the above solution describes the system geometry: two superposed liquid-gas layers with the liquid boundary at $z=0$, the gas boundary at $z=2$, and the diffuse interface around $z=1$. The fluids being incompressible and the interface rigid, the system configuration given by the relation (5) doesn't change, that means we don't need in this model a spatiotemporal evolution equation for the density. Starting from an initial random pattern we show in Fig. 1 some

two-dimensional (x, z) snapshots for the stream-function till formation of the convective pattern and reaching of the saturation state. Although explicit interface conditions were not imposed in our formalism, one remarks in Fig. 1 the appearance of the liquid-gas interface in an early stage of evolution at $t = 75$ s. Concomitantly two convective motions develop: one in the liquid and the second one in the gas, when the gradient temperature exceeds a critical value.

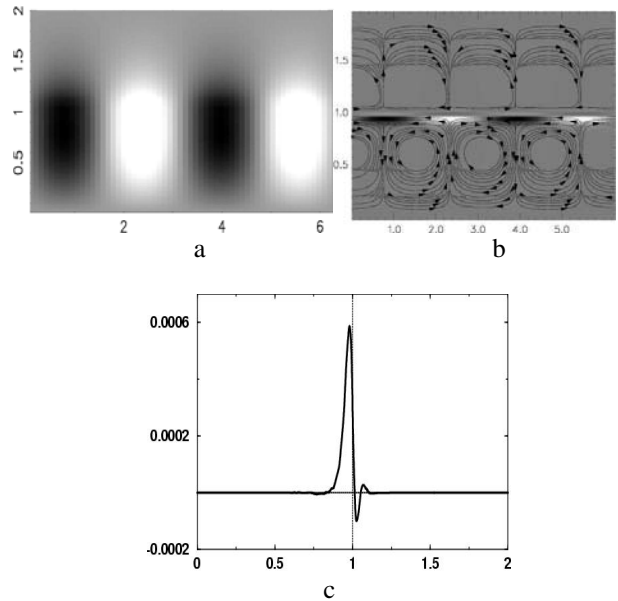


Fig. 2. Temperature perturbations (panel (a)), stream-lines and density perturbations (panel(b)) induced by the thermo-capillary instability. Panels (a) and (b) illustrate two-dimensional (x, z) perturbation profiles and the panel (c) illustrates the density perturbation versus z in the rising liquid. The plots come from the model with compressible fluids and deformable interface and correspond to a water-air system heated from below.

Model 2: compressible fluids with deformable interface.

A more realistic model considers the fluids compressible and the interface deformable. In this case no stream function exists. We compute the stream-lines directly from the velocity components and the spatiotemporal evolution of the density from the mass continuity equation. The panels from Fig. 2 illustrate the temperature perturbations, the stream-lines and the density perturbations for Marangoni convection driven by the thermo-capillary effect. The pictures from Fig. 2 are gathered after a long time interval when the saturation state is already achieved. With all these pictures done, one can explain now the trigger mechanism of this convective instability. So, increasing the temperature difference top-bottom over a threshold – which depends on the system geometry – temperature patterns emerge in the whole liquid-gas system as shown in Fig. 2-a. The surface tension coefficient decreases usually with temperature so that at the liquid-gas interface turn up regions with lower and higher surface tension coefficient. Along the interface appear surface-tension-driven forces (called “Marangoni forces”) which push the fluid from regions with lower

surface tension (light regions in Fig. 2-a) to regions with larger surface tension (dark regions in Fig. 2-a). In this way above and below the interface cellular rolls arise as one can see in Fig. 2-b. Fig. 2-c plots the density perturbations ρ_1 (against z) caused by the surface-tension-driven instability in the rising liquid. Convection in liquid pushes the liquid against the interface which leads to an increase of the density at the interface on the liquid side. The advection of gas from the top plate creates a lower density at the interface. Consequently two peaks appear in (z, ρ_1) representation given by Fig. 2-c, which are asymmetrical because the density in the liquid is much larger than the density in the gas state.

Model 3: compressible evaporating fluids. We include now in the previous model evaporation/condensation phenomena in the interfacial region. The double-well potential (2) which describes the free-energy density has to become now asymmetrical in the disturbed states of the two-layer system. In this way one of the phases (liquid or gas) becomes locally more stable than the second one, fact which allows for interfacial mass exchange between the two phases. We model this relative vertical shift of the minima (of the free-energy density) by adding in the relation (2) a supplementary term:

$$f(\rho, T) = f_0(\rho) + r(\rho - 1)(T - T_0(z)) \quad (6)$$

where $T_0(z)$ represents the temperature distribution of the system in stationary conditions and r is a bias parameter related to the specific latent heat L (for more details about this model see [10]).

On the other side in the classical heat equation has to appear a supplementary term of phase field describing the jump of normal heat fluxes due to latent heat:

$$\rho c \frac{dT}{dt} = \nabla \cdot (\kappa \nabla T) + L \frac{\partial \rho}{\partial t} \quad (7)$$

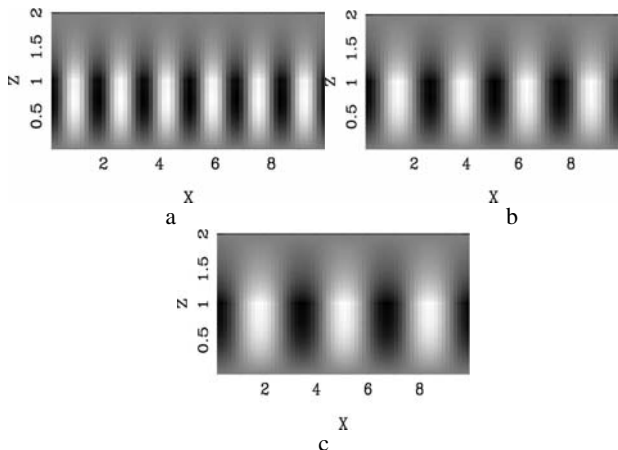


Fig. 3. Patterns for temperature perturbation in ethanol-vapor system heated from below as it results from model 3. The external heating is kept constant and the latent heat is increased: (a) $L = 700$ kJ/kg; (b) $L = 3800$ kJ/kg; (c) $L = 4150$ kJ/kg.

We fix the temperature gradient far above the threshold and we change the latent heat varying r and L . Fig. 3 plots the perturbed temperature field for ethanol-vapor parameters corresponding to different L . Experimentally, the latent heat L is modified by covering the liquid-vapor interface with different mono-layers surfactants. So, increasing the latent heat the number of the convection cells on the same lateral length decreases from 6 to 3. Actually, the change of the number of cells means a change of the excited mode in the liquid-vapor system. That reveals a phenomenon already experimentally confirmed [11]: far from threshold there appear interesting options to *control* the *wavelength* of the convective rolls by the *latent heat*.

4. Conclusions

In summary, we developed phase field models for Marangoni convection in two-layer systems with external heating. Starting from Lagrangian formalism we found out a supplementary term of phase field which has to be included in Navier-Stokes equation in order to substitute the boundary conditions from the classical models. Non-linear simulations were shown coming out from models with incompressible and compressible fluids. Extending the phase field model to compressible evaporating fluids we analyzed the influence of the evaporation on the convective patterns.

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