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# THE BEHAVIOR OF UNSTEADY THERMOCAPILLARY FLOWS

David R. Vrane and Marc K. Smith  
The George W. Woodruff School of Mechanical Engineering  
Georgia Institute of Technology  
Atlanta, Georgia

## ABSTRACT

The thermocapillary-driven flow of a liquid in a shallow slot provides a simple model to explore the effects of free-surface deflection and end walls on the stability of the flow. Such an investigation may be useful in understanding the complex flow seen in processes such as the float-zone refining of single crystals. A linear stability analysis of the viscously-dominated slot flow indicates stable basic states to both two- and three-dimensional infinitesimal disturbances for capillary numbers below 43.3. Above this capillary number steady solutions do not exist. We also discuss current work involving the development of an inertially-dominated slot-flow model using singular perturbation methods. If these flows are unstable, inertial effects would be the only possible cause of the instability.

## INTRODUCTION

Thermocapillary flows are driven by temperature-induced surface tension gradients at the interface between two immiscible fluids. For most liquids, the surface tension decreases with increasing temperature. Thus, when the interface experiences a positive temperature gradient the bulk fluids on each side of the interface must balance an effective negative shear stress. Through this mechanism, the thermal fields in the fluids are coupled to the velocity fields.

One important process in which thermocapillary flows are seen is the float-zone processing of crystalline materials. Here, an amorphous rod of semiconducting material passes through a ring heater producing a local melt-zone along the rod. Ideally, as the material travels past the heater, the leading portion of the molten material solidifies and forms a single, uniform crystal. However, since the conditions at the freezing end of the zone dictate the uniformity of the material, the presence of unsteady thermocapillary flows in the melt-zone can compromise crystal quality.

The present work describes the first two of a series of analytical models designed to isolate the mechanisms that cause thermocapillary-driven flows in finite regimes, such as the float zone, to become time dependent. The basic model, originally investigated by Sen and Davis (1), is the flow in a single liquid layer bounded by two end walls. This geometry is also called the flow in a shallow slot. Sen and Davis (1) provided a steady, asymptotic solution (small depth to width ratios) for a viscously-dominated flow in the slot with first-order surface deflections. Sen (2) extended this analysis to leading-order surface deflections. In our current work, we find that steady solutions for the flow are only possible for capillary numbers below 43.3. A linear stability analysis shows that these steady solutions are stable to both two- and three-dimensional infinitesimal disturbances. In our second flow model, we consider an inertially-dominated flow in the slot in an effort to investigate the role of fluid inertia on the instability of the slot flow. Previous work by Smith and Davis (3) has shown that fluid inertia plays a significant role in the stability mechanism for long wavelength surface wave instabilities.

## ANALYSIS

In the earlier work of Sen and Davis (1) and Sen (2), hereafter referred to as SD and Sen respectively, the authors analyzed thermocapillary flows in a rectangular slot of aspect ratio  $A$ , defined as the depth of the fluid layer over the width of the slot, in the limit  $A \rightarrow 0$ . Their analyses

were based on the assumption that the Reynolds and Marangoni numbers were both  $O(A)$ . However, SD considered capillary numbers of  $O(A^4)$  while Sen looked at capillary numbers of  $O(A^3)$ . The former scaling resulted in nearly parallel flows in the core matched to return flows in the end layers with only small corrections to the flat interface. The latter scaling produced nonparallel core flows with  $O(1)$  surface deflections. The present work focuses on the stability of the results found in Sen, but will make frequent references to the derivations originally developed in SD.

Written in stream function form, the dynamics of the fluid within the cavity are described by the following dimensionless equations (see SD for notation):

$$RA\left[\left(\psi_{yyt} + \psi_y\psi_{xyy} - \psi_x\psi_{yyy}\right) + A^2\left(\psi_{xxt} + \psi_y\psi_{xxx} - \psi_x\psi_{xyy}\right)\right] \\ = \psi_{yyyy} + 2A^2\psi_{xyy} + A^4\psi_{xxxx} \quad (1a)$$

$$MA\left[T_t + \psi_y T_x - \psi_x T_y\right] = T_{yy} + A^2 T_{xx}. \quad (1b)$$

The dimensionless boundary conditions are given by

$$x = \pm \frac{1}{2}: \psi_x = \psi_y = 0, T = \mp \frac{1}{2} \quad (2a)$$

$$y = 0: \psi_x = \psi_y = 0, T_y = 0 \quad (2b)$$

$$y = h(x, t): h_t = -\psi_y h_x - \psi_x \quad (2c)$$

$$-p + 2A^2(1 + A^2 h_x^2)^{-1} \left[ (-\psi_{xy} - h_x \psi_{yy}) + A^2 h_x (\psi_{yy} + h_x \psi_{xy}) \right] \quad (2d)$$

$$= A^3 C^{-1} h_{xx} (1 + A^2 h_x^2)^{-3/2} (1 - A^{-1} CT)$$

$$(1 - A^2 h_x^2)(\psi_{yy} - A^2 \psi_{xx}) - 4A^2 h_x \psi_{xy} = -(1 + A^2 h_x^2)^{1/2} (T_x + h_x T_y) \quad (2e)$$

$$(1 + A^2 h_x^2)^{-1/2} (T_y - A^2 h_x T_x) + L(T + x) = 0. \quad (2f)$$

The constant-volume condition is given by

$$\int_{-1/2}^{1/2} h(x, t) dx = 1, \quad (3a)$$

and for steady flow, a zero mass-flux condition holds across the depth of the fluid

$$\int_0^{h(x)} \psi_{oy}(x, y) dy = \psi_o(h(x)) - \psi_o(0) = 0. \quad (3b)$$

Finally, for the case where the ends of the interface are of fixed height, we impose

$$h(\pm \frac{1}{2}) = 1. \quad (4)$$

For the viscously-dominated flow, Sen took  $R = \bar{R}A$ ,  $M = \bar{M}A$ , and  $C = \bar{C}A^3$ , where the overbarred terms are all  $O(1)$ . In the limit  $A \rightarrow 0$ , the core flow was derived by expanding the dependent variables of the system in terms of an asymptotic series in  $A$ . Substituting these expansion into equations (1-4), and solving the leading-order system in terms of  $h(x)$ , Sen obtained the following approximations for the stream function and the interface position in the core

$$\psi_o(x, y) = \frac{1}{4} y^2 \left[ \frac{y}{h(x)} - 1 \right] \quad (5)$$

$$h_o h_{xxx} = -3\bar{C} / 2. \quad (6)$$

At both end walls, the leading-order, inner systems required that the interface remain flat throughout the boundary-layers, making equation (6) valid across the entire slot and subject to the pinned-end conditions (4).

In the current work, equation (6) was solved using a Chebyshev pseudo-spectral method in conjunction with a Newton-Kantorovich iteration scheme. The results of these computations are shown in figure 1 for several values of the capillary number. Steady interface solutions were found in the range  $0 \leq \bar{C} \leq 43.3$ . For capillary numbers above this limit, the Newton-Kantorovich scheme failed to converge, perhaps indicating the existence of unsteady basic-states. Further investigation of this behavior near this limit and for even larger capillary numbers still remains to be done.

We determined the stability to three-dimensional small disturbances of this viscously-dominated system by perturbing the steady interface as follows

$$h(x, z, t) = H(x) + \hat{h}(x) e^{s + \alpha z}, \quad (7)$$

where  $H(x)$  is the steady interface solution,  $\hat{h}(x)$  is the disturbance mode shape,  $s$  is the disturbance growth rate, and  $\alpha$  is the disturbance wave number transverse to the flow direction. Note that for two dimensional disturbances  $\alpha = 0$ . Substituting equation (7) into the stream function equation (5) and the three-dimensional form of the kinematic equation (2c), substituting equation (5), evaluated at the interface, into equation (2c), and then linearizing yields the general linearized disturbance interface equation

$$s\hat{h} = \frac{1}{2} (H_x + H\hat{h}_x) - \frac{H^2}{3\bar{C}} (3H_x(\hat{h}_{xxx} - \alpha^2\hat{h}_x) + H(\hat{h}_{xxxx} - 2\alpha^2\hat{h}_{xx} + \alpha^4\hat{h})), \quad (8)$$

subject to the conditions

$$x = \pm \frac{1}{2}: \hat{h} = \hat{h}_{xxx} = 0 \quad (9a,b)$$

$$\int_{-1/2}^{1/2} \hat{h}(x, t) dx = 0. \quad (10)$$

Condition (9b) is the perturbation form of the zero volume flux condition (3b), which becomes restricted to the endwalls for unsteady flow.

The system of equations (8-10) presents an eigenvalue problem in  $s$  that was solved using a Chebyshev spectral method in combination with an IMSL eigenvalue routine. The results of these computations are shown in figure 2. Here, the most dangerous growth rate is plotted against its respective capillary number for various wave numbers. Note that all of the disturbance growth rates are negative for the viscously-dominated flow, signifying that the steady solutions of this flow model are always stable. In addition, for any capillary number, transverse disturbances have a stabilizing effect. Finally, it is interesting that for two-dimensional disturbances the growth rate approaches zero as the capillary number approaches the upper limit for the existence of steady-flow solutions.

Since the viscously-dominated slot is unconditionally stable to small disturbances, there will be no doubt as to the origin of resulting instabilities when new effects are added to the model. In our second model, we add the effect of fluid inertia. This addition is accomplished by changing the

Reynolds number scaling from  $R = \bar{R}A$  to  $R = \bar{R}A^{-1}$ . Physically, this means that we have gone from considering an  $O(1)$  Prandtl number fluid to an  $O(A^2)$  Prandtl number fluid. Such a rescaling may provide a better approximation to the thermocapillary flows of low Prandtl number fluids such as liquid silicon. Substituting this scaling into equations (1) and (2) yields the following leading-order, core-flow system

$$R[\psi_{oyyt} + \psi_{oy}\psi_{oxy} - \psi_{ox}\psi_{oyy}] = \psi_{oyyy} \quad (11a)$$

$$T_{oyy} = 0 \quad (11b)$$

$$y=0: \psi_{ox} = \psi_{oy} = 0, T_{oy} = 0 \quad (12a)$$

$$y = h_o(x, t): h_{ot} = -\psi_{oy}h_{ox} - \psi_{ox} \quad (12b)$$

$$-p_o = \bar{C}^{-1}h_{xxx} \quad (12c)$$

$$\psi_{oyy} = -(T_{ox} + h_{ox}T_{oy}) \quad (12d)$$

$$T_{oy} + L(T_o + x) = 0. \quad (12e)$$

Clearly, the solution of this system will require a numerical approach, but it is still far simpler than the full Navier-Stokes equations. Fortunately, since the thermal field remains conduction-dominated to leading order, the inner conditions still require a flat interface in the end layers. Therefore, the leading-order outer solution may be obtained by solving for the interface position and stream function simultaneously subject to the additional conditions

$$\int_{-1/2}^{1/2} h_o(x, t) dx = 1 \quad (13a)$$

$$\int_0^{h(x)} \psi_{oy}(x, y) dy = \psi_o(h(x)) - \psi_o(0) = 0 \quad (13b)$$

$$h(\pm \frac{1}{2}) = 1. \quad (13c)$$

The numerical approach used to solve this system of equations will employ a double iteration scheme as follows. Using the leading-order solution provided by Sen as an initial guess, a spectral, Newton-Kantorovich scheme will be used to solve the nonlinear equation (11a) subject to conditions (12a, b, d) and (13b). This will provide an intermediate solution for the stream function. The intermediate solution will then be used to calculate the pressure field from the  $x$ -momentum equation. Once the pressure is known, condition (12c) may be integrated subject to conditions (13a, c) to give a corrected interface shape. This process is repeated until both the stream function and the interface shape converge to a solution.

## FUTURE PLANS

Once the inertially-dominated flow has been computed and explored with regard to its stability, we wish to explore other effects that can be easily incorporated into this slot-flow model. These effects can be summarized with the following model problems.

(1) A flat, annular geometry in which the flow is in the radial direction and the transverse direction is periodic. In this model we shall explore the effect of the geometric deceleration of the flow as it moves radially outward from the center. The interface itself remains relatively flat for small capillary numbers. This geometry is also relevant to the space flight experiment of Ostrach (4).

(2) A vertical, annular geometry in which the flow is in the vertical direction and the transverse direction is periodic. With this model, we include the capillary pressure associated with the curvature of the interface in this cylindrical geometry. Such curvature has the potential to balance the stabilizing effect of surface tension seen in the original flat-slot model.

(3) A cylindrical geometry. Here, we let the inner wall of the annular geometry go to zero and obtain a long capillary bridge. This geometry is the most relevant to the float-zone geometry, but it still keeps the end effects as only a boundary condition on the flow in the core.

With these three model problems, we shall explore a variety of effects that can contribute to the instability of the thermocapillary flow. The advantage of using this succession of models is that the individual effects are included one at a time. This will allow an unambiguous study of their relative effect on the stability. Such a treatment may succeed in identifying the underlying mechanism of the thermocapillary instabilities seen in these systems.

In each model, we shall consider a viscously-dominated and an inertially-dominated flow field. Once the numerical codes are developed to handle the inertial problem in the original flat-slot geometry, the inclusion of the effects represented in the other models is relatively straightforward.

## CONCLUSION

By constructing a series of models that successively includes more and more effects, this research will seek to clarify the roles of both fluid inertia and flow geometry in contributing to the nature of the instabilities seen in thermocapillary flows. The viscously- and inertially-dominated slot models addressed in this paper are just the first two models in this series.

We have found that the viscously-dominated flow in the flat-slot geometry has steady, two-dimensional solutions for capillary numbers less than 43.3, and that these solutions are stable to both two- and three-dimensional infinitesimal disturbances. The inertially-dominated flow problem has been posed and is now in the process of numerical code development.

## ACKNOWLEDGMENTS

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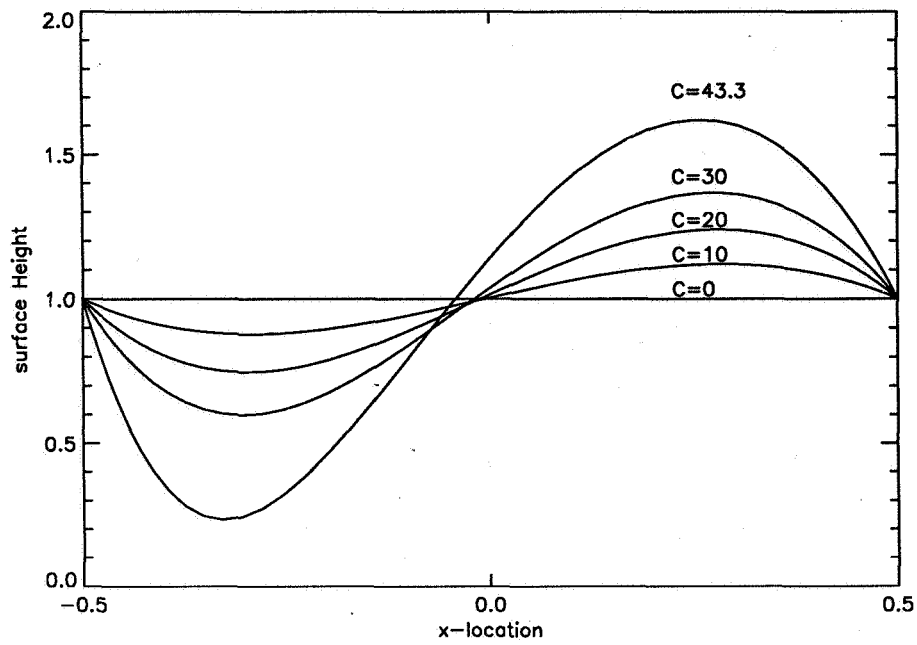


Figure 1 – The interface shape for various values of the scaled capillary number  $\bar{C}$ .

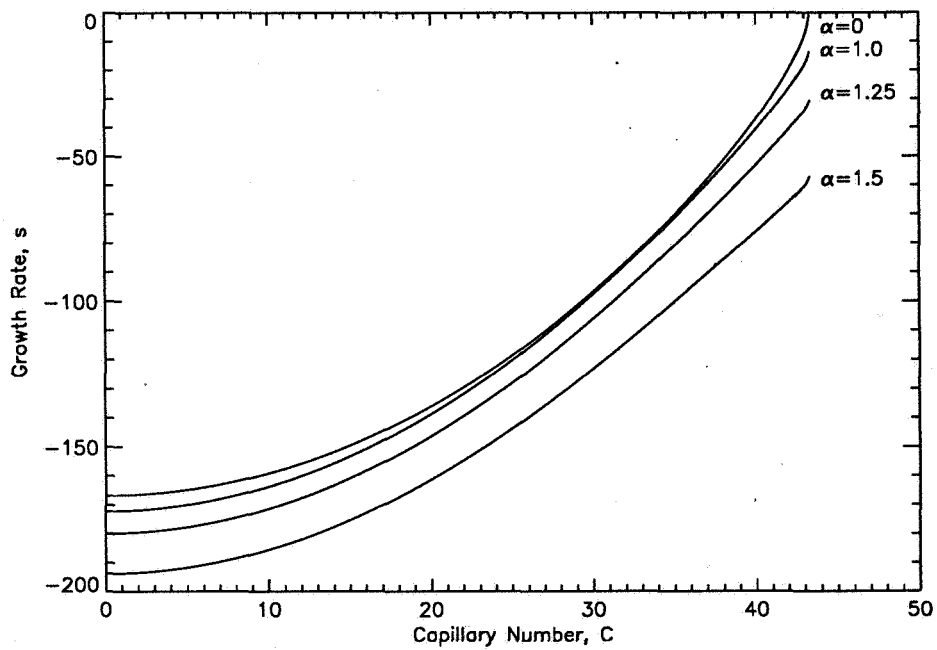


Figure 2 – The growth rate as a function of the scaled capillary number  $\bar{C}$  for various values of the wave number  $\alpha$ .