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Objective function choice for control of a thermocapillary flow using an adjoint-based control strategy

Frank H. Muldoon *, Hendrik C. Kuhlmann

Institute of Fluid Mechanics and Heat Transfer, Vienna University of Technology, Resselgasse 3, A-1040 Vienna, Austria

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ABSTRACT

The problem of suppressing flow oscillations in a thermocapillary flow is addressed using a gradient-based control strategy. The physical problem addressed is the "open boat" process of crystal growth, the flow in which is driven by thermocapillary and buoyancy effects. The problem is modeled by the two-dimensional unsteady incompressible Navier–Stokes and energy equations under the Boussinesq approximation. The goal of the control is to suppress flow oscillations which arise when the driving forces are such that the flow becomes unsteady. The control is a spatially and temporally varying temperature gradient boundary condition at the free surface. The control which minimizes the flow oscillations is found using a conjugate gradient method, where the gradient of the objective function with respect to the control variables is obtained from solving a set of adjoint equations. The issue of choosing an objective function that can be both optimized in a computationally efficient manner and optimization of which provides control that damps the flow oscillations is investigated. Almost complete suppression of the flow oscillations is obtained for certain choices of the objective function.

1. Introduction

One goal behind mathematical or experimental modeling of fluid and heat transfer problems is the design or control of engineering systems. Such design or control inherently carries with it the concept of optimization, as the goal is to select control inputs or design parameters such that the engineering system is *optimal* according to a prescribed metric. Optimization of engineering systems does not require a mathematical model of the system, however, the existence of such a model can greatly aid optimization in two ways. One way is a much shorter time with which a solution satisfying the mathematical model can often be obtained compared to that required to carry out experiments. The other is that a mathematical model potentially can contain information such as derivatives and sensitivities with respect to the quantities being varied that are very difficult, if not practically impossible, to obtain from experiments. The numerical methods used in the area of Computational Fluid Dynamics to obtain approximate solutions to mathematical models such as the Navier–Stokes and energy equations and computing resources have advanced to a stage where many fluid and heat-transfer problems of engineering interest may be reliably solved quickly enough that they can be used in all stages of the design cycle. This has enabled Computational Fluid Dynamics to replace expensive physical prototype models and has greatly reduced design cost and time. This corresponds to the first way that mathematical modeling can aid optimization, in which the mathematical model is used as a "drop in" replacement for experimental models. A more efficient means of using a mathematical model is its combination with an optimization method which uses higher order information about the physical system such as derivatives that can be obtained from the mathematical model.

A field with a high demand of optimization is crystal growth. A major problem in crystal-growth processes with a free surface is the appearance of microscopic striations which are the results of impurity segregation. The striations arise due to unsteadiness in the growth process at the crystallization front which can arise from temperature fluctuations in the molten material (Müller and Ostrogorsky, 1994). Flow and temperature fluctuations, despite time-independent boundary conditions, are typically due to instabilities of the flow which is driven by thermocapillary and buoyancy forces which cannot be avoided. Thermocapillary surface forces arise along the interface (free surface) between the molten material and the surrounding atmosphere due to the thermocapillary effect which is caused by the dependence of the surface tension on temperature (Kuhlmann, 1999).

The goal of the present work is to investigate issues involved with combining a mathematical model of the unsteady Navier–Stokes and energy equations with an optimization method with the aim of controlling a thermocapillary flow including the

* Corresponding author.
E-mail address: fmuldoo@me.lsu.edu (F.H. Muldoon).

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Nomenclature

α	distance along line in search direction
Γ	aspect ratio, horizontal over vertical distance
ϕ	control variables
$\phi_{\max}(\phi_{\min})$	maximum (minimum) value of the control variables
Ω	the spatial computational domain
$\partial\Omega$	the boundary of Ω
$\partial\Omega_{\mathrm{fs}}$	the part of $\partial\Omega$ containing the free surface, $\partial\Omega_{\mathrm{fs}} \subseteq \partial\Omega$
H	objective function used by the minimizer
H_p	penalty part of objective function
h	vertical distance
p	pressure
T	temperature
t	time
t_{EH}	event horizon length
t_A	temporal advancement length, the extent of the temporal dimension of ϕ, $t_A \leqslant t_{EH}$
$\boldsymbol{u}$	velocity vector
u	first component of velocity vector (i.e., u_1)
v	second component of velocity vector (i.e., u_2)
x	spatial coordinate in horizontal direction
y	spatial coordinate in vertical direction

temperature field that is a model of a manufacturing process for crystals. The control in question is a spatially and temporally varying normal temperature gradient at the free surface of the thermocapillary flow. The objective is to find control that suppresses an unsteady flow due hydrodynamic instabilities which arise for Reynolds numbers greater than a certain critical value. The time scales of slightly supercritical thermocapillary flows are much larger than those of high-Reynolds-number turbulent flows. This makes them an ideal target for real-time control, since the time available to carry out the computations needed to find optimal control over some period of time will be substantially smaller than the real (wall clock) time available to carry out the computations. Note, however, that real crystal growth is much more complicated than the model flow studied here (se e.g. Hurle, 1994). Therefore, our study of a very much simplified model flow can only be a first step towards a real industrial application.

A literature review concerning the combination of optimization/control with Computational Fluid Dynamics in general exists in Muldoon (2013). To avoid repetition, we briefly mention here only the work on thermocapillary flows. Thermocapillary systems that have been the subject of investigation of flow control are thermocapillary liquid layers (as a model for the open-boat technique) and thermocapillary half-zones (as a model for the floating-zone technique). Benz et al. (1998) measured the free-surface temperature variation caused by flow oscillations in thermocapillary liquid layers. They have experimentally proven the feasibility of suppressing these oscillations by heating the free surface along lines parallel to the isolines of constant phase of the oscillations. In a series of papers Shiomi and co-workers have experimentally demonstrated the feasibility of feedback control of thermocapillary flows by suppression of oscillations in an annular pool resembling the Czochralski process (Shiomi et al., 2001; Shiomi and Amberg, 2002) and in the half zone-model model of the floating-zone technique (Shiomi et al., 2003). In all experiments temperature signals were recorded from two sampling points on the free surface and the control was applied by point heating the free surface at one or two other points. For the annular pool, Shiomi and Amberg (2005) confirmed their experimental results by simulating some representative cases.

In the present work we consider the control of the two-dimensional thermocapillary flow in an open boat. In contrast to previous investigations we make use of the full information provided by the free surface temperature and control is applied at the whole free surface. In a work closely related to the present work Muldoon (2013) demonstrated control of flow oscillations in this geometry. The mathematical model, the two-dimensional unsteady incompressible Navier–Stokes equations and energy equations, was the same as in the present work. It was found that the length of the "event horizon" (i.e., the distance ahead in time over which optimal control was found), played a significant role in the success of finding control that suppressed the flow oscillations. The present work represents a continuation of Muldoon (2013) focusing on investigation of different objective functions and issues involved with solving the optimization problems required to determine the optimal control.

The present work uses a conjugate-gradient algorithm to find optimal control. Such a method requires the gradient of the objective function to be minimized with respect to the control input. Therefore, a key issue is the means by which this gradient is obtained. In the present work this gradient is obtained by solving an additional set of adjoint equations derived from the governing mathematical model. Aside from gradient-based optimization methods, there exist methods such as simulated annealing and genetic algorithms that do not require a gradient (Davis, 1987). Such methods are very useful if the gradient of the objective function cannot be obtained or does not exist, but since they lack the information about the function being minimized contained in the gradient, they typically require many more evaluations of the objective function than gradient-based methods. This represents a serious disadvantage for the solution of the mathematical problem considered in the present work, which, as it involves solving the unsteady Navier–Stokes and energy equations over time periods of significant length, is extremely expensive to compute. In the present work, the computational expense in terms of arithmetical operations required for computing the gradient by means of solving the adjoint equations is similar to that required to compute the objective function. For this reason, a gradient-based optimization method is a more efficient approach for optimization for the present problem.

2. Formulation of the problem

A schematic with dimensions and boundary conditions of the physical system to be investigated is given in Fig. 1. This system is known as an "open boat" in the literature. The problem contains a free surface, at which, due to gradients in the surface tension

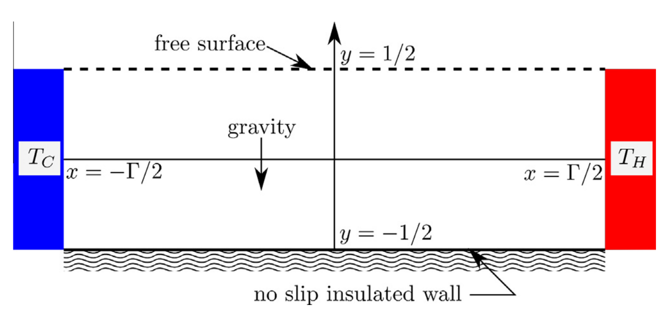

Fig. 1. Schematic of physical domain for the minimization problem showing boundary conditions and dimensions.