AN ADJOINT METHOD FOR THE INVERSE DESIGN OF SOLIDIFICATION PROCESSES WITH NATURAL CONVECTION

GEORGE Z. YANG AND NICHOLAS ZABARAS *
Sibley School of Mechanical and Aerospace Engineering, 188 Frank H. T. Rhodes Hall, Cornell University, Ithaca, NY 14853-3801 U.S.A.

ABSTRACT

This paper presents a finite element algorithm based on the adjoint method for the design of a certain class of solidification processes. In particular, the paper addresses the design of directional solidification processes for pure materials such that a desired freezing front heat flux and growth velocity are achieved. This is the first time that an infinite-dimensional continuum adjoint formulation is obtained and implemented for the solution of such inverse/design problems with moving boundaries and Boussinesq incompressible flow.

The present design problem belongs to a category of inverse problems in which one is looking for the unknown conditions in part of the boundary, while overspecified boundary conditions are supplied in another part of the boundary (here the freezing interface). The solidification design problem is mathematically posed as a whole time-domain optimization problem. The gradient of the cost functional is calculated using the solution of an appropriately defined continuous adjoint problem. The minimization process is realized by the conjugate gradient method via the solutions of the direct, adjoint and sensitivity sub-problems.

The proposed methodology is demonstrated with the solidification of an initially superheated liquid aluminum confined in a square mold. The non-uniformity in the casting product in the direction of gravity due to the existence of natural convection in the melt is emphasized. The inverse design problem is then posed as finding the appropriate spatial-temporal variations of the boundary heat flux on the vertical mold walls that can eliminate or reduce the effects of convection on the freezing interface heat fluxes and growth velocity. The numerical example demonstrates the accuracy and convergence of the adjoint formulation. Finally, open related research design problems are discussed. © 1998 John Wiley & Sons, Ltd.

KEY WORDS: inverse problems; adjoint equations; solidification; natural convection; design optimization; uniformity in casting products

1. INTRODUCTION

In solidification processes, the melt flow can be invoked by buoyancy effects from temperature-dependent density variations. The temperature in the solid and liquid regions, the velocity field of the liquid melt, and the solid–liquid interface location history are well defined as long as the temperature (or heat flux) are specified on the whole exterior boundary of the solid–liquid domain.

* Correspondence to: Nicholas Zabaras, Sibley School of Mechanical Engineering, Cornell University, 188 Frank H. T. Rhodes Hall, Ithaca, NY 14853-3801, U.S.A. E-mail: njz1@cornell.edu

Contract/grant sponsor: National Science Foundation; Contract/grant numbers: DDM-9157189 and CTS-9115438

This mathematical problem constitutes what we usually refer to as the direct problem of solidification. Conditions of existence, uniqueness and stability are well documented for such well-posed problems.

On the other hand, various design solidification problems take the form of an inverse problem in which incomplete conditions are available in part of the boundary, whereas overspecified boundary conditions have been supplied in another part of the boundary or inside the domain. Inverse problems are ill-posed and the existence, uniqueness and stability of their solution is not guaranteed. Even though the ill-posedness makes inverse design problems challenging both theoretically and numerically, the practical importance of inverse problem theory-based designs has led to extensive research efforts. Most of the attention has been given to conduction-based inverse heat transfer problems because of the simplicity of the governing equations and due to the significant number of engineering applications. Inverse conduction-based solidification problems were also addressed with emphasis on the design and control of the mold cooling/heating conditions such that a desired solid–liquid interface morphology is achieved. Solution techniques such as the time sequential method, the whole time-domain method, including finite- and infinite-dimensional optimization schemes, were developed to calculate the unknown functions. The infinite-dimensional optimization method, also known as the functional optimization method, requires the formulation of an appropriate continuum adjoint problem that makes the analytical calculation of the gradient of the cost functional feasible. Such adjoint methods for inverse heat conduction problems are well established.

Some attention to inverse heat transfer problems involving free or forced convection has also been given. The adjoint method has been used to study such problems without a dynamic coupling of the thermal and fluid flow fields. In our recent work, we derived a functional optimization formulation and continuum adjoint equations for inverse natural convection problems with linearly coupled temperature and velocity fields through the buoyancy force. The adjoint problem was defined such that the values of the adjoint thermal field on the boundary with unknown boundary conditions was equal to the gradient of an appropriately defined cost functional in the $L_2$ space. Note that the adjoint thermal field was dynamically coupled with the adjoint flow field similarly to the thermal/fluid flow coupling in the direct natural convection problem. Reference 18 presented the analysis of various inverse natural convection problems in fixed domains. For each problem examined, a unique solution was shown to exist that corresponded to a zero cost functional.

In this study, we are extending the formulation of Reference 18 to the design of directional solidification processes with natural convection that results in desired freezing front heat fluxes and growth velocity. In particular, the design objectives include the interface growth velocity, $v_n$, or equivalently the history of the interface geometry $\Gamma(t)$, and the heat flux history $q_l$ in the liquid side of the interface. Both $v_n$ and $q_l$ are spatial and temporal functions.

Our motivation considers the fact that the combination of $v_n$ and $q_l$ dictates the type and scale of the microstructures in the final cast product. The presence of natural convection has profound effects on the spatial distribution of $v_n$ and $q_l$, and thus it dynamically influences the homogeneity of the final cast product. It is beyond the scope of this paper to discuss details about such microstructural implications in solidification processing, though our choice of particular inverse design objectives relies heavily on such important physical arguments.

Our earlier work considered only an inverse conduction problem in the solid phase mainly because the interface growth velocity was the only design objective. When the thermal flux $q_l$ at the interface also becomes an additional design objective, two inverse problems, one in the...
solid phase and another in the liquid phase need to be solved. These problems are separable and only related through the Stefan condition on the interface location. In this paper, the inverse problem in the solid phase is identical to that studied in Reference 11. As such, emphasis here will only be given to the inverse problem in the liquid phase, which is an inverse convection problem on a time-dependent domain with coupled thermal and melt flow fields.

In Section 2, a generic definition of the direct solidification problem is presented to set forward the notation for the inverse analysis.

The definition of the inverse solidification design problem is given in Section 3. The numerical procedure includes the solution of the continuum direct, adjoint and sensitivity sub-problems as required by the conjugate gradient optimization scheme. The derivations of the adjoint equations for the inverse convection problem on a time-dependent domain are outlined in the Appendix. The finite element method is used for the solution of the direct, sensitivity and adjoint problems.

Section 4 includes the numerical examples, some implementation details and the obtained results. An example problem of the solidification of liquid aluminum in a square mold is set up to demonstrate the effects of convection on the interface shape and interface heat distribution. We select the desired interface objectives to be the same as those obtained in a related solidification process but without convection (i.e. in a one-dimensional two-phase Stefan problem). The inverse convection solidification problem is then defined as follows: Adjust the mold cooling/heat conditions corresponding to an initial design such that in the presence of convection the interface heat and growth velocity are as close as possible to the desired interface objectives. Since no exact solution to this inverse problem has been known or shown to exist, the emphasis here is in the calculation of a local minimum of a proper cost functional that provides a design that is a substantial improvement over the initial design. The accuracy and convergence characteristics of the inverse design algorithm are also examined and physical implications are discussed.

Finally, the present work is summarized and suggestions for future research are made in Section 5.

2. THE DIRECT SOLIDIFICATION PROBLEM WITH NATURAL CONVECTION

Here, we introduce in a parametric form the direct directional solidification problem for pure materials. The present model will provide the foundation for the definition of the inverse design problem to be given in the next section. Consider a two-dimensional domain \( \Omega \) initially occupied by the liquid melt of a pure substance. Solidification starts at time \( t = 0^+ \) and proceeds as shown in Figure 1. For \( t > 0 \), \( \Omega \) is divided into the solid region \( \Omega_s \) and the liquid region \( \Omega_l \). These regions are separated by a moving solid-liquid interface \( \Gamma_1 \). The boundaries of \( \Omega_s \) and \( \Omega_l \) are denoted as \( \Gamma^s \) and \( \Gamma^l \), respectively. They are sub-divided as \( \Gamma^s = \Gamma_q \cup \Gamma_h^s \cup \Gamma_1 \) and \( \Gamma^l = \Gamma_o \cup \Gamma_h^l \cup \Gamma_1 \) as shown in Figure 1. The subscripts \( h \) and \( q \) are used to denote boundaries with specified heat flux and temperature, respectively, whereas the subscript \( o \) is here used to define a boundary where a heat flux \( q_o \) is applied. The heat flux \( q_o \) and temperature \( \theta_o \) are considered to be functional parameters to the direct problem in the sense that we are interested to evaluate the temperature and velocity fields \( T(x,t;q_o,\theta_o) \) and \( v(x,t;q_o,\theta_o) \), respectively, for various heat fluxes \( q_o \) and temperatures \( \theta_o \), while maintaining the remaining of the boundary conditions on \( \Gamma_h^s \) and \( \Gamma_h^l \) fixed.

Subscripts \( s \) and \( l \) distinguish properties or field quantities of the solid and liquid phases. Also, the reference temperature is denoted as \( T_1 \), while the freezing temperature as \( T_m \). Let \( L \) be the problem characteristic length, \( \rho \) the density, \( c \) the specific heat, \( K \) the thermal conductivity, \( \alpha \) the diffusivity, \( \beta \) the thermal expansion coefficient, \( \sigma \) the surface tension, \( \gamma \) the viscosity and \( \varepsilon \) the thermal diffusivity. The symbols \( \epsilon \) and \( \sigma \) represent the electrical conductivity and the thermal conductivity, respectively.
Figure 1. The direct solidification problem

The direct solidification problem is considered here, where the thermal diffusivity \( \alpha = K / \rho c \) and \( \nu \) the kinematic viscosity. All thermophysical quantities are assumed to be constants. The time scale is chosen as \( L^2 / \nu \). We also define the dimensionless temperature as \( \theta = (T - T_m) / (T_i - T_m) \), the dimensionless velocity as \( \mathbf{u} = \nu \mathbf{L} / \nu \) and the dimensionless pressure as \( p = PL^2 / \rho \nu^2 \), where \( P \) is the actual dynamic pressure.

The thermal transfer of the solidification process considered here is modelled as conduction in the solid region \( \Omega_s \), conduction and natural convection in the liquid region \( \Omega_L \), and latent heat (denoted by \( L \)) release at the solid-liquid interface \( \Gamma \). The convective melt flow is modelled by the incompressible Navier–Stokes equations, in which the buoyancy force is subjected to density variations following the Boussinesq approximation. Laminar flow assumption is made and the viscous dissipation is neglected. The key dimensionless parameters involved are: the Stefan number \( \text{Stef} = c_r (T_i - T_m) / \nu \), the Prandtl number \( \text{Pr} = \nu / \alpha \) and the Rayleigh number \( \text{Ra} = g \beta (T_i - T_m) L^3 / \nu \), where \( \beta \) is the thermal expansion coefficient of the liquid melt.

In the direct solidification problem with \( q_o \) as a parameter, the dimensionless governing equations for the liquid region \( \Omega_L \) are

\[
\frac{\partial \theta_L(x, t; q_o, \theta_g)}{\partial t} + \mathbf{u}(x, t; q_o, \theta_g) \cdot \nabla \theta_L(x, t; q_o, \theta_g) = \nabla^2 \theta_L(x, t; q_o, \theta_g) \tag{1}
\]

\[
\frac{\partial \mathbf{u}(x, t; q_o, \theta_g)}{\partial t} + [\nabla \mathbf{u}(x, t; q_o, \theta_g)] \mathbf{u}(x, t; q_o, \theta_g) = -\nabla p(x, t; q_o, \theta_g) + \text{Pr} \nabla^2 \mathbf{u}(x, t; q_o, \theta_g) - \text{Ra} \text{Pr} \theta_L(x, t; q_o, \theta_g) \mathbf{e}_g \tag{2}
\]

\[
\nabla \cdot \mathbf{u}(x, t; q_o, \theta_g) = 0 \tag{3}
\]

where \( \mathbf{e}_g \) is the unit vector in the direction of gravity. The corresponding initial and boundary conditions are

\[
\theta_L(x, 0; q_o, \theta_g) = \theta_i(x), \quad x \in \Omega_L \tag{4}
\]

\[
\mathbf{u}(x, 0; q_o, \theta_g) = 0, \quad x \in \Omega_L \tag{5}
\]

\[
\mathbf{u}(x, t; q_o, \theta_g) = 0, \quad (x, t) \in \Gamma^l \times [0, t_{\text{max}}] \tag{6}
\]

© 1998 John Wiley & Sons, Ltd.

where \( n \) denotes the unit outer normal of the boundary of the domain involved.

The dimensionless governing equation for the solid region is

\[
R_s \frac{\partial \theta_s(x, t; q_o, \theta_g)}{\partial t} = \nabla \cdot (R_s \nabla \theta_s(x, t; q_o, \theta_g))
\]

where \( R_s = \frac{\rho c_s}{\rho c_f} \) and \( R_k = \frac{K_s}{K_f} \). The boundary conditions for the solid phase are as follows:

\[
\theta_s(x, t; q_o, \theta_g) = \theta_g(x, t), \quad (x, t) \in \Gamma_g \times [0, t_{max}]
\]

\[
\frac{\partial \theta_s(x, t; q_o, \theta_g)}{\partial n} = q_s(x, t), \quad (x, t) \in \Gamma_s \times [0, t_{max}]
\]

The latent heat release at the moving solid–liquid interface is described by the following Stefan condition:

\[
\text{Ste}^{-1} v_f \cdot n = R_k \frac{\partial \theta_s(x, t; q_o, \theta_g)}{\partial n} - \frac{\partial \theta_f}{\partial n}(x, t; q_o, \theta_g), \quad x \in \Gamma_1
\]

where \( v_f \) is the velocity of the solid–liquid interface. Thermodynamic equilibrium requires an isothermal freezing interface:

\[
\theta_f(x, t; q_o, \theta_g) = \theta_m(x, t; q_o, \theta_g) = \theta_m, \quad x \in \Gamma_1
\]

For each heat flux \( q_o \) on \( \Gamma_o \) and temperature \( \theta_g \) on \( \Gamma_g \), equations (1)-(13) define a well-posed problem that can be solved for the solid and liquid temperature fields, the melt velocity field and the normal velocity \( v_f \cdot n \) of the interface.

This direct solidification problem is solved by a front tracking Petrov Galerkin finite element method, with a deforming mesh. The incompressibility condition (3) is written as follows:

\[
p = -\chi \nabla \cdot \mathbf{u}
\]

where \( \chi \) is the penalty number. The above condition is numerically handled by the consistent penalty method. The weak formulations, FEM matrix equations and time stepping scheme are the same as those in Reference 18, while the mesh motion is handled as in Reference 24. Some more finite element implementation details will be provided in Section 4.

3. THE INVERSE DESIGN SOLIDIFICATION PROBLEM AND THE ADJOINT FORMULATION

3.1. Definition of the inverse design problem

Let us consider a fixed domain \( \Omega \) that initially contains a quiescent liquid melt of a pure material at temperature \( \theta_i \). The notation remains the same as that introduced in the previous section. Known boundary conditions are assumed to be applied on the boundaries \( \Gamma_s \) and \( \Gamma_g \). We assume that solidification starts at time \( t = 0 \) on the left wall boundary and that the freezing front
\( \Gamma(t) \) propagates to the right under conditions of natural convection (see Figure 1). In addition to the above known flux conditions, we also desire that solidification occurs with prescribed thermal and growth conditions at the boundary \( \Gamma(t) \). In particular, we assume:

1. a desired solid-liquid interface \( \Gamma(t) \) moving with a known normal velocity \( \bar{v}_n \)
2. a desired interfacial heat flux history \( \frac{\partial \theta_s}{\partial n} = \bar{q}_1 \) on \( \Gamma(t) \).

Note that a set of overspecified conditions are provided on the boundary \( \Gamma(t) \) (heat flux \( \bar{q}_1 \) and the melting temperature \( \theta_m \)). The main unknowns of the above inverse problem are then the temperature condition on \( \Gamma \) and the heat flux history on \( \Gamma \).

Since the interface location history \( \Gamma(t) \) is given, the above inverse problem can be separated into two inverse sub-problems, one in the solid phase and another in the liquid melt. The two problems are briefly defined as follows:

1. In the solid region \( \Omega_s \), with equations (9), (11) and (13), and the extra boundary condition:
   \[
   \frac{\partial \theta_s}{\partial n} = \bar{q}_1 + Ste^{-1}\bar{v}_n, \quad \text{on } \Gamma
   \]  
   find the thermal boundary conditions (here the temperature \( \theta_s \)) on \( \Gamma \).
2. In the liquid region \( \Omega_l \), with equations (1)-(7) and (13), and the extra boundary condition
   \[
   \frac{\partial \theta_l}{\partial n} = \bar{q}_1 \quad \text{on } \Gamma
   \]  
   find the thermal boundary conditions (here the heat flux \( q_l \)) on \( \Gamma \).

In both problems, in addition to the freezing temperature \( \theta_m = 0 \), a heat flux condition is supplied on the interface \( \Gamma \). In the solid phase, the flux \( \frac{\partial \theta_s}{\partial n} \) (equation (15)) together with the condition of equation (11) and the governing equation (9) are used to define a parametric problem for each temperature \( \theta_s \) on \( \Gamma \). The temperature field solution to this problem is denoted as \( \theta(x, t; \theta_s) \) (i.e. \( \theta_s \) is the only functional parameter to this direct conduction problem). The solution \( \bar{\theta}_s \) of the inverse problem in the solid phase is then defined by the minimization with respect to \( \theta_s(x, t) \in L_2(\Gamma \times [0, t_{\text{max}}]) \) of the following functional:

\[
S_s(\theta_s) = \frac{1}{2} \| \theta_s(x, t; \theta_s) - \theta_m \|^2_{L_2(\Gamma \times [0, t_{\text{max}}])}
= \frac{1}{2} \int_0^{t_{\text{max}}} \int_{\Gamma} \left[ \theta_s(x, t; \theta_s) - \theta_m \right]^2 d\Gamma dt
\]  

A similar inverse heat conduction problem, with data \( \frac{\partial \theta_l}{\partial n} \) (equation (15)) provided through the solution of a direct natural convection problem, was studied earlier in Reference 11. As such, the above inverse/design heat conduction problem will not be further discussed in this paper. Note that in Reference 11 an unknown heat flux was considered on the left wall. The choice of unknown temperature in this paper was only made to simplify the presentation of the example problem to be presented later in Section 4. The inverse convection problem in the melt can also be stated as an optimization problem. With a guessed \( q_o \) in equation (8) and using equations (1)-(8) and (16), one can define a direct problem on the prescribed liquid domain \( \Omega_l \). The solution of this natural convection problem is denoted as \( \bar{\theta}_l(x, t; q_o) \) to emphasize that \( q_o \) is the only needed parameter. One can restate the calculation of the quasi-solution \( \bar{q}_o \in L_2(\Gamma \times [0, t_{\text{max}}]) \) of the inverse problem in the liquid phase.
as the minimization of the following cost functional with respect to \( q_0(\mathbf{x}, t) \in L_2(\Gamma_0 \times [0, t_{\text{max}}]) \):

\[
S_f(q_0) = \frac{1}{2} \left\| \frac{\partial}{\partial\Gamma}(\mathbf{x}, t; q_0) - \theta_m \right\|_{L_2(\Gamma_1 \times [0, t_{\text{max}}])}^2
= \frac{1}{2} \int_0^{t_{\text{max}}} \int_{\Gamma_1} \left[ \frac{\partial}{\partial\Gamma}(\mathbf{x}, t; q_0) - \theta_m \right]^2 d\Gamma dt
\tag{18}
\]

Note that for this inverse natural convection problem, the field \( \frac{\partial}{\partial\Gamma}(\mathbf{x}, t; q_0) \) is calculated simultaneously with the flow field \( \mathbf{u}(\mathbf{x}, t; q_0) \). Also, note that the cost functional is defined over the whole time domain, i.e. from \( t = 0 \) to \( t_{\text{max}} \) (maximum time of interest). The cost functional \( S \) measures the discrepancy between the calculated temperature \( \theta(\mathbf{x}, t; q_0) \) at \( \Gamma_1(t) \) and the given interface temperature \( \theta_m \). In summary, the inverse problem in the liquid phase can be formulated as the following functional minimization problem:

**Find the optimal boundary heat flux** \( \tilde{q}_0(\mathbf{x}, t), (\mathbf{x}, t) \in (\Gamma_0 \times [0, t_{\text{max}}]) \) (equation (8)), such that

\[
S_f(\tilde{q}_0) \leq S_f(q_0), \quad \forall q_0 \in L_2(\Gamma_0 \times [0, t_{\text{max}}])
\tag{19}
\]

where \( S_f \) is given by equation (18), in which \( \theta \) is defined through equations (1)–(8) and (16).

To simplify the notation, we will remove from now on the subscript \( \ell \) from all field variables referring to the liquid phase and for example denote \( \theta \) as \( \theta \). Due to the implicit dependence of \( S_f \) on \( q_0 \) through the complicated governing equations, it is an open mathematical task to rigorously establish the equivalence between the solution of the above optimization problem and \( S_f = 0 \) which implies satisfying the inverse design objectives exactly. Certain compatibility conditions are generally required between the given data \( \theta_m, q_0 \), the material properties and geometry in order for a solution of the inverse problem to exist with \( S_f(\tilde{q}_0) = 0 \). In this paper, our objective is to construct a minimizing sequence \( q_k^0(\mathbf{x}, t) \in L_2(\Gamma_0 \times [0, t_{\text{max}}]), k = 1, 2, \ldots \) that converges to at least a local minimum of \( S_f(q_0) \). This is sufficient from a designer’s point of view in the sense that generally one does not expect to be able to achieve arbitrary interfacial data (heat flux and growth velocity) by solely adjusting the thermal boundary conditions on \( \Gamma_0 \).

3.2. Formulation of the adjoint method and the optimization scheme

To perform the optimization procedure that minimizes \( S_f(q_0) \) in \( L_2(\Gamma_0 \times [0, t_{\text{max}}]) \), we will need to define a sensitivity problem. This linear problem defines the linear perturbations \( \Theta(x, t; q_0, \Delta q_0) \equiv D_q\theta(x, t; q_0) \) and \( \mathbf{U}(x, t; q_0, \Delta q_0) \equiv D_qu(x, t; q_0) \) of the fields \( \theta(x, t; q_0) \) and \( \mathbf{u}(x, t; q_0) \), respectively, with respect to variations \( \Delta q_0(x, t) \) of the boundary heat flux \( q_0 \), i.e.

\[
\begin{align*}
\theta(x, t; q_0 + \Delta q_0) &= \theta(x, t; q_0) + \Theta(x, t; q_0, \Delta q_0) + O(\left\| \Delta q_0 \right\|_{L_2(\Gamma_0 \times [0, t_{\text{max}}])}^2) \\
\mathbf{u}(x, t; q_0 + \Delta q_0) &= \mathbf{u}(x, t; q_0) + \mathbf{U}(x, t; q_0, \Delta q_0) + O(\left\| \Delta q_0 \right\|_{L_2(\Gamma_0 \times [0, t_{\text{max}}])}^2)
\end{align*}
\tag{20, 21}
\]

Linearization of the direct problem in the liquid phase results in the following continuum sensitivity problem (recall that the subscript \( \ell \) is dropped from the various fields to simplify the notation):

\[
\begin{align*}
\frac{\partial}{\partial t} \Theta(x, t; q_0, \Delta q_0) + \mathbf{u}(x, t; q_0) \cdot \nabla \Theta(x, t; q_0, \Delta q_0) + \mathbf{U}(x, t; q_0, \Delta q_0) \cdot \nabla \theta(x, t; q_0) \\
= \nabla^2 \Theta(x, t; q_0, \Delta q_0)
\end{align*}
\tag{22}
\]
\[
\frac{\partial U(x, t; q_o, \Delta q_o)}{\partial t} + [\nabla U(x, t; q_o, \Delta q_o)] \frac{\partial u(x, t; q_o)}{\partial t} + [\nabla u(x, t; q_o)] U(x, t; q_o, \Delta q_o)
\]

\[
= -\nabla \Pi(x, t; q_o, \Delta q_o) + Pr \nabla^2 U(x, t; q_o, \Delta q_o) - Pr Ra \Theta(x, t; q_o, \Delta q_o) \mathbf{e}_g
\]

(23)

\[
\Pi(x, t; q_o, \Delta q_o) = -\lambda \nabla \cdot U(x, t; q_o, \Delta q_o)
\]

(24)

\[
\Theta(x, 0; q_o, \Delta q_o) = 0, \quad x \in \Omega_f
\]

(25)

\[
U(x, 0; q_o, \Delta q_o) = 0, \quad x \in \Omega_f
\]

(26)

\[
U(x, t; q_o, \Delta q_o) = 0, \quad (x, t) \in \Gamma' \times [0, t_{\text{max}}]
\]

(27)

\[
\frac{\partial \Theta}{\partial n}(x, t; q_o, \Delta q_o) = 0, \quad (x, t) \in (\Gamma_0 \cup \Gamma_1) \times [0, t_{\text{max}}]
\]

(28)

\[
\frac{\partial \Theta}{\partial n}(x, t; q_o, \Delta q_o) = \Delta q_o(x, t), \quad (x, t) \in \Gamma_0 \times [0, t_{\text{max}}]
\]

(29)

where \(\Pi\) is the sensitivity pressure and \(\lambda\) is the same penalty number as that used in equation (14).

In order to realize the minimization of \(S_t(q_o)\), it is essential to find its gradient (derivative) with respect to \(q_o\). Using the definition of \(S_t(q_o)\) we can see that the exact gradient \(S_t'(q_o)\) of the cost functional in the \(L_2(\Gamma_0 \times [0, t_{\text{max}}])\) space satisfies the following integral relation:

\[
\int_0^{t_{\text{max}}} \int_{\Gamma_0} S_t'(q_o(x, t)) \Delta q_o(x, t) \mathrm{d}\Gamma \mathrm{d}t = \int_0^{t_{\text{max}}} \int_{\Gamma_1} \Theta(x, t; q_o, \Delta q_o)(\theta(x, t; q_o) - \theta_m) \mathrm{d}\Gamma \mathrm{d}t
\]

(30)

The above-equation implies that the exact gradient calculation requires the derivation of an appropriate adjoint to the operator of the thermal sensitivity operator. After some lengthy but straightforward calculations (see the appendix as well as Reference 9 for similar derivations in fixed domains), the following adjoint problem is defined:

\[
\frac{\partial \psi(x, t; q_o)}{\partial t} + u(x, t; q_o) \cdot \nabla \psi(x, t; q_o) = -\nabla^2 \psi(x, t; q_o) + \phi(x, t; q_o) \cdot \mathbf{e}_g
\]

(31)

\[
\frac{\partial \phi(x, t; q_o)}{\partial t} + [\nabla \phi(x, t; q_o)] u(x, t; q_o) - [\nabla u(x, t; q_o)]^T \phi(x, t; q_o) = \nabla \pi(x, t; q_o)
\]

\[= -Pr \nabla^2 \phi(x, t; q_o) + Pr Ra \psi(x, t; q_o) \nabla \theta(x, t; q_o)
\]

(25)

\[
\pi(x, t; q_o) = -\lambda \nabla \cdot \phi(x, t; q_o)
\]

(33)

\[
\psi(x, t_{\text{max}}; q_o) = 0, \quad x \in \Omega_f
\]

(34)

\[
\phi(x, t_{\text{max}}; q_o) = 0, \quad x \in \Omega_f
\]

(35)

\[
\phi(x, t; q_o) = 0, \quad (x, t) \in \Gamma' \times [0, t_{\text{max}}]
\]

(36)

\[
\frac{\partial \psi}{\partial n}(x, t; q_o) = 0, \quad (x, t) \in (\Gamma_0' \cup \Gamma_0) \times [0, t_{\text{max}}]
\]

(37)

\[
\frac{\partial \psi}{\partial n}(x, t; q_o) - (v_t \cdot n) \psi(x, t; q_o) = \theta(x, t; q_o) - \theta_m, \quad (x, t) \in \Gamma_1 \times [0, t_{\text{max}}]
\]

(38)

where \(\psi(x, t; q_o)\) is the adjoint temperature, which is coupled with an adjoint velocity field \(\phi(x, t; q_o)\). Also, \(\pi\) is the adjoint pressure and \(\lambda\) is the same penalty number as that used in equation (14).

As part of the derivation of the adjoint system and using equation (30), one can show (see Appendix) that the exact gradient of the cost functional is given as follows:

\[
S_t'(q_o(x, t)) = \psi(x, t), \quad (x, t) \in \Gamma_0 \times (0, t_{\text{max}})
\]

(39)
We have outlined above the definition of the continuous direct, adjoint and sensitivity problems. The Conjugate Gradient Method (CGM) can now be used for the minimization of the cost functional $S(q_0)$. It constructs a sequence: $q_0^0, q_0^1, \ldots, q_0^n, \ldots$, to approach the optimal minimizer $q_0^*$.

The procedure is the following:

**Step A:** Make an initial guess of $q_0^0(x, t) \in L_2(\Gamma_0 \times [0, t_{\text{max}}])$ and set $k = 0$.

**Step B:** Calculate the conjugate search direction $p^k(x, t)$, $(x, t) \in \Gamma_0 \times [0, t_{\text{max}}]$:

1. Solve the direct problem for $\theta(x, t; q_0^k)$ and $u(x, t; q_0^k)$.
2. Compute the residual $(\theta(x, t; q_0^k) - \theta_m)$ for $(x, t) \in \Gamma_1 \times [0, t_{\text{max}}]$.
3. Evaluate $S(q_0^k)$ from equation (18); If $S(q_0^k) < \varepsilon$ (given tolerance), set $q_0^* = q_0^k$ and stop.
4. Solve the adjoint problem backwards in time for $\psi(x, t; q_0^k)$.
5. Set $S'(q_0^k) = \psi(x, t; q_0^k)$.
6. Set $r^k = 0$, if $k = 0$; otherwise:

$$r^k = \frac{(S'(q_0^k), S'(q_0^{k-1}) \big|_{L_2(\Gamma_0 \times [0, t_{\text{max}}])})}{\|S'(q_0^{k-1})\|^2_{L_2(\Gamma_0 \times [0, t_{\text{max}}])}}$$

7. Define $p^k(x, t)$, if $k = 0$, $p^0 = -S'(q_0^k)$; Otherwise, $p^k = -S'(q_0^k)(x, t) + r^k p^{k-1}$.

**Step C:** Calculate the optimal step size $\alpha^k$:

1. Solve the sensitivity problem for $\Theta(x, t; q_0^k, p^k)$ and $U(x, t; q_0^k, p^k)$.
2. Calculate $\alpha^k$ by

$$\alpha^k = \frac{-(S'(q_0^k), p^k)_{L_2(\Gamma_0 \times [0, t_{\text{max}}])}}{\|\Theta(x, t; q_0^k, p^k)\|^2_{L_2(\Gamma_0 \times [0, t_{\text{max}}])}}$$

**Step D:** Update $q_0^{k+1}(x, t) = q_0^k(x, t) + \alpha^k p^k(x, t)$, $(x, t) \in \Gamma_0 \times [0, t_{\text{max}}]$

**Step E:** Set $k = k + 1$ and go to Step B.

The inner product in the $L_2$ space involved in the CGM procedure is defined as:

$$(f, g)_{L_2(\Gamma_0 \times [0, t_{\text{max}}])} = \int_0^{t_{\text{max}}} \int_{\Gamma} f g \, d\Gamma \, dt$$

4. NUMERICAL IMPLEMENTATION, RESULTS AND DISCUSSION

In this section, we will consider a directional solidification example problem with convection and we will briefly discuss the effects of convection on the freezing interface morphology (Section 4.1). We will then address the design problem of modifying the boundary flux conditions such that the effects of convection on the interface morphology are minimized (Section 4.3). In particular, our desired solution is to obtain interfacial conditions that are as close as possible to those corresponding to the case of pure conduction, i.e. to a two-phase Stefan problem (Section 4.2). Finally, Section 4.4 presents a validation of the proposed design as well as discussion on the obtained results.

4.1. The direct solidification problem with convection

We consider a directional solidification process for pure liquid aluminum confined in a square mold of dimensionless side length 1 (see Figure (2a)). The liquid melt is initially at a uniform...
temperature $T_i = 860\degree C$. The top, bottom and right walls are kept adiabatic. From $t = 0^+$, the
temperature of the left vertical wall ($x = 0$) is dropped below the freezing temperature $T_m =
660\degree C$, to the room temperature $T_o = 25\degree C$ and maintained at that temperature for $t > 0$. The
thermophysical properties are taken the same as those used in Reference 24 and result in the
following dimensionless quantities: $Pr = 0.0149$, $Ste = 0.5317$, and $Rc = Rk = 1$. The Rayleigh
number used is $1.6 \times 10^4$. The dimensionless wall cooling temperature in equation (10) is constant,
\[ \theta_g = (T_o - T_m)/(T_i - T_m) = -3.175. \] The initial liquid melt is at $\theta_{\text{init}} = 1$ in equation (4) and the
dimensionless freezing temperature $\theta_m = 0$ by definition. The dimensionless heat fluxes $q'_h$ in
equation (7), $q_o$ in equation (8), and $q'_h$ in equation (11) all become zero from the adiabatic mold
wall conditions.

The penalty number in equation (14) is taken as $\lambda = 10^8$. A fixed number of $20 \times 20$ quadrilateral linear elements are used in each of the material phases (Figure 3). Let $(s(y,t), y)$ denote a
point on the solid–liquid interface $\Gamma_1$ at time $t$. Taking advantage of the directional nature of the
solidification process, we make the choice of the freezing interface velocity to be
\[ \mathbf{v}_f = \left(\frac{\partial s}{\partial t}\right)\mathbf{e}_x, \]
where $\mathbf{e}_x$ is the unit vector in the $x$-direction. This means that we force the interface nodes to
move horizontally. It is important to emphasize that the energy balance on the interface (i.e. the
Stefan condition given by equation (12)) controls only the normal to the interface motion. Our
choice of horizontal $\mathbf{v}_f$ implies that a tangential motion to the interface is superimposed to its
normal motion determined by the Stefan condition. Based on the selected interface motion, the
finite element mesh is forced to deform linearly in the $x$-direction, i.e., the mesh velocity is
selected as follows:

\begin{align*}
\mathbf{v}_m(x,y,t) & = \frac{x}{s(y,t)} \frac{\partial s}{\partial t} \mathbf{e}_x, \quad (x,y) \in \Omega_s \quad \text{(41)} \\
\mathbf{v}_m(x,y,t) & = \frac{1-x}{1-s(y,t)} \frac{\partial s}{\partial t} \mathbf{e}_x, \quad (x,y) \in \Omega_l \quad \text{(42)}
\end{align*}

Let $n_x = \mathbf{n} \cdot \mathbf{e}_x$. Noting that the boundary line segment $d\Gamma = dy/n_x$, we can simplify the weak
form of the Stefan condition as follows (the general treatment of the Stefan condition is reviewed
in Reference 24):

\[ Ste^{-1} \left\{ \int_{\Gamma_1} N^i N^j \, dy \right\} \mathbf{v}'_f = \int_{\Gamma_1} N^i \left\{ R_k \frac{\partial \theta_s}{\partial n} - \frac{\partial \theta_f}{\partial n} \right\} \, d\Gamma \quad \text{(43)} \]

where $N^i$ are the shape functions and $i$, $j$ are nodal indices. This form of the weak Stefan
condition can be used to calculate the (horizontal) nodal velocities $v_f$. The right-hand side of the
above equation is calculated directly from the discretized energy equations corresponding to the
nodes on $\Gamma_1$. A constant time step $\Delta t = 0.001$ is selected with $t_{\text{max}} = 0.5$ when approximately
96 per cent of the initial liquid melt has solidified.

The resultant transient temperature and velocity fields, interface location $s(y,t)$ and interfacial
heat flux $q_1 = (\partial \theta_f/\partial n)(s,y,t)$, etc., will be presented in Section 4.4 in comparison with the results
corresponding to the optimal inverse design. In order to clarify the following discussions, from
now on we will refer to the solution of the present direct solidification problem with convection
(Figure 2(a)) as the initial design.
4.2. The direct solidification problem without convection

In the above direct convection-based solidification example (Figure 2(a)), the onset of natural convection results in a curved solid–liquid interface \( \partial s/\partial y \neq 0 \), as well as in a vertical non-uniformity of the interfacial heat flux \( \partial q_l/\partial y \neq 0 \). If we neglect natural convection \( Ra = 0 \), the problem of section 4.1 is reduced to a one-dimensional two-phase Stefan problem on a finite domain\(^28\) (Figure 2(b)). Using the same numerical scheme as before, the solution of the interface location \( s_r(t) \) and the interface heat flux \( q_r(t) \) for this Stefan problem have been calculated and are shown in Figure 4. This solution is used to define the desired design objectives of our inverse...
analysis and from now on we will refer to it as the desired design solution (even though it is only the interfacial quantities of this solution that we are interested on). From Figure 4, we observe that \( q_r \approx 0 \) at \( t > 0.36 \). This indicates that after some time, the desired design solution behaves like that corresponding to a one-phase Stefan problem. The effect of the finite liquid region is responsible for the nearly constant slope \( \dot{s}_r(t) \) at the later stages of solidification.\(^{28}\)

The definitions of the initial design and desired design solutions are introduced to emphasize that our design objective is here going to be the control of the temperature \( \theta_y \) in \( \Gamma_g \) and flux \( q_o \) in \( \Gamma_o \) in the case of solidification with convection such that the resulting interface growth and interfacial heat fluxes are identical to those in the absence of convection (i.e. as close as possible to the desired design solution presented in Figure 4).

4.3. Solution of the example inverse design problem

The adjoint method formulation presented in Section 3.2 is hereby implemented for the inverse design problem introduced at the end of Section 4.2. More specifically, the design problem is stated as follows:
Find the thermal condition on the left wall \( x = 0 \) and the right wall \( x = 1 \) such that with natural convection in the melt, a vertical interface \( x = s_r(t) \) and a vertically uniform interfacial heat flux \( q_l = q_r(t) \) are achieved.

Here, \( s_r(t) \) and \( q_r(t) \) are exactly the same as the data given in Figure 4, whereas the remaining of the boundary conditions of the design problem are the same as those used in the initial design problem of Figure 2(a). Figures 2(c) and (d) give the complete definition of the two inverse/design subproblems, the one in the solid phase (Figure 2(c)) and the other in the liquid melt (Figure 2(d)). The thermophysical properties are identical to those of the initial design problem of Figure 2(a) as presented in Section 4.1. Thus, the inverse problem is simply the elimination of the effects of natural convection on the freezing interface’s morphology and local temperature gradients. Since \( v_n \) and \( q_l \) are the main macroscopic variables that control the obtained solidification microstructures, we can also state that the inverse design objective is to achieve the same final cast product as the one obtained without natural convection in the melt. This work represents preliminary attempts for flow control and we have intentionally kept the strength of convection at moderate levels \( (Ra = 1.6 \times 10^4) \).

The solution of the inverse problem in the solid phase (Figure 2(c)) is automatically known from the boundary condition of the initial design problem, \( \theta_y = -3.175 \) at \( x = 0 \), which is also the boundary condition of the Stefan problem shown in Figure 2(b). An inverse heat conduction problem in the solid region could be solved to validate the above solution. It is of no interest to this paper to check the accuracy of the inverse heat conduction problem in the solid phase as such problems were examined earlier.7–11 Thus, we will concentrate on the solution of the inverse design problem in the liquid phase alone (Figure 2(d)).

The inverse problem in the liquid solves for \( q_o(y,t) \) at \( x = 1 \) with given freezing interface location \( s_r(t) \) and heat flux \( q_r(t) \) and the other mold walls being adiabatic. An initial guess \( q_o^0(y,t) = 0 \) is taken (this corresponds to the initial design of Figure 2(a)). The CGM algorithm is essentially a local optimization scheme and as such we expect that the CGM converges to a local minimizer associated with the initial guess solution \( q_o^0(y,t) = 0 \).

The time domain \([0, t_{\text{max}}]\) is taken with \( t_{\text{max}} = 0.36 \). With this choice, convection will practically be very weak at time \( t_{\text{max}} \), and thus the adjoint method’s end condition difficulty based on the current initial guess will not be important (see Reference 11 for discussion on the importance of \( q_o^0(y,t_{\text{max}}) \) to the convergence of the adjoint CGM algorithm). No prominent convection effects need to be compensated by \( q_o(y,t) \) at \( t > t_{\text{max}} \) and thus we expect that the optimal solution will satisfy \( \tilde{q}_o(y,t > t_{\text{max}}) \equiv 0 \). Also note that the choice of \( t_{\text{max}} \) affects the required computational efforts as well as the convergence rate.

Within each CGM iteration, the direct, adjoint and sensitivity problems are solved with the same finite element algorithm as in the direct solidification problem. The spatial and temporal discretizations remain the same for all three problems (for related numerical implementation details see Reference 18). The cost of each CGM iteration including the solutions of the three subproblems is about half an hour CPU time on an IBM RS-6000 workstation. The convergence of the CGM method is shown in Figure 5. The cost functional \( S_r \) decreases monotonically with the number of the CGM iterations. After about 60 iterations, a much slower reduction of \( S_r \) is observed. As in similar iterative regularization methods,5 a cut-off iteration \( \tilde{k} = 200 \) is selected based on a tolerance of \( \varepsilon = 3 \times 10^{-5} \), which corresponds to \( S_r(q_o^{200}) \sim 10^{-2}S_r(q_o^0) \). The spatial and temporal variations of the optimal solution \( \tilde{q}_o = q_o^{200}(y,t) \) are shown in Figure 6. The optimal solution exhibits the largest amount of heating and cooling at the corners of \( x = 1 \) and at the earlier
stages of solidification. This is expected as the boundary heat flux $q_o$ should be adjusted early in time so that at later times it can influence the convection effects on the freezing interface. Note that a certain amount of time is required before variations in the $y$-direction and time of the heat flux $q_o$ can be felt in the calculated temperature $\theta$ at the freezing interface. This required time is higher at earlier times when the interface $x = s(y, t)$ is at a further distance from the wall $x = 1$. After $t = 0.3$, $\tilde{q}_o(y, t)$ starts to approach zero. This indicates that our a priori choices of $t_{\text{max}} = 0.36$ and $q_0(0, t_{\text{max}}) = 0$ were appropriate in avoiding the end condition difficulty characteristic of adjoint methods. Finally, Figure 7 presents the calculated heat fluxes $q_k^o$ at various intermediate CGM iterations.

4.4. Validation of the inverse design solution

To evaluate how close the design objectives (i.e. the data of Figure 4) have been met, we consider a direct solidification problem (including the simultaneous analysis of the solid and liquid
phases) with the optimal heat flux $\tilde{q}_o(y, t)$ applied at $x = 1$, $\theta_x = -3\cdot175$ at $x = 0$ and the remaining walls kept adiabatic. We call the solution to this problem the inverse optimal design solution. We will here compare this inverse design solution and that of the initial design and report the deviation of the obtained interface growth velocity and heat fluxes from the desired values of Figure 4.

In order to quantify the achievement of vertical uniformities of the interface heat flux and growth velocity, the following two standard deviations are defined for the inverse design objectives $s$ and $q_I$:

$$
\sigma_s(t) = \left\{ \int_0^1 [s(y, t) - s_r(t)]^2 \, dy \right\}^{1/2}
$$

$$
\sigma_{q_I}(t) = \left\{ \int_0^1 [q_I(y, t)/n_x(y, t) - q_r(t)]^2 \, dy \right\}^{1/2}
$$

Figure 7. Flux solution $q_o(y, t)$ at intermediate iterations: (a) 25; (b) 50; (c) 100; (d) 150
Figure 8 shows the time histories of $s(x,t)$ and $q_I(x,t)$ for the optimal and initial designs. The maximum of $s(t)$ throughout the whole time history is reduced by a factor of about 8, whereas the maximum of $q_I$ is reduced by a factor of 4. The inverse design results in a solution that satisfies better the vertically flat interface condition rather than the vertically uniform heat flux condition. The vertical non-homogeneity of $q_I$ and of the interface velocity $v_f$ are comparable mainly due to the way the Stefan condition was implemented in the direct analysis (equation (12)). Considering that the front location is calculated by integration over time of the front velocity, it will be natural to expect a front shape that is smoother than the growth velocity. At earlier stages of solidification, the solid and dashed lines overlap (Figure 8). This implies that the inverse design adjustment at $x = 1$ can do little to cure the vertical non-uniformity of the interface quantities at the early stages of solidification. This is expected since the ill-posedness of the problem is higher at the early times when the wall $x = 1$, where the flux $q_o$ is applied, is the furthest apart from the freezing interface. The moment of maximum of $s(t)$ is close to the time that convection is strongest, while the peak of $s(t)$ comes at a later time. At the later stages of solidification and due to the directional solidification nature of this example problem, the convection effects are weakened and the vertical interface non-uniformities relax to zero values. To further visualize the extent of the vertical uniformity of the design objectives, some contour lines are plotted on the whole physical domain of solidification: Figure 9(a) shows the interface position at different indicated times and Figure 9(b) shows the contour lines of the interface heat flux $q_I$. For comparison, the dashed lines are also introduced to indicate the initial design solution. Note that in Figure 9(b), the value of a contour line passing through a point $(x, y)$ is referring to the interface heat flux $q_I$ when the interface passed through that point. The $x$-locations at which the design objectives are most vertically nonuniform, correspond to the desired interface locations at the times of occurrence of the peaks in Figure 8.

It is rather of interest to examine similar contour lines of another combined quantity $q_I/v_n$, which decides the refinement of the solidification microstructures without changing the morphology. The uniformity of $q_I/v_n$ in the present example will imply a $y$-uniformity of the solidification morphology for each $x$ slice in the final cast product. The contour lines for $q_I/v_n$ are presented in Figure 10 on the right for the solution based on the inverse design and on the left for the initial design solution. The labelled lines have the corresponding values of $q_I/v_n$ tabulated to the right. At earlier time, such lines are vertical for both cases since no significant convection has yet been
Figure 9. Comparisons of the optimal interface location \( x = \alpha(y; t) \) and heat flux \( q_1(y; t) \) contours with those corresponding to the initial design solution.

Figure 10. Comparison of the vertical uniformity of the production condition \( q_1/v_u \) in the final casting product for the initial and optimal designs developed. The inverse solution achieves nearly vertical uniformity of \( q_1/v_u \) at later stages since by then convection has been drastically reduced. In the middle region of the casting product, the inverse design solution is able to remove a 'hot island' at the top region of the initial design solution.

The temperature fields in the solid and liquid phases as well as the flow field in the liquid are displayed in Figures 11 and 12 for representative times \( t = 0.05, 0.12, 0.22, \) and \( 0.32 \). Contour of isotherms and of the stream function \( \psi \) represent the temperature and flow field, respectively, for both the inverse design solution (right) and the initial design solution (left). Extreme temperature and stream function values are given on the top of each contour plot at the various times.

The thermal field with the optimal design always has the bottom corner at $x = 1$ as the hottest spot. Cooling generally is happening in the middle region of $x = 1$ while the upper corner at $x = 1$ is a heat sink at earlier stage and a weaker source than the bottom corner later. This directly relates to the spatial as well as temporal behaviour of $q_o(y,t)$ which is shown in Figure 6. The distribution of isotherms near $x = 1$ influences the shape of the isotherms in the liquid region near the interface, and makes them vertical and equally spaced to achieve the vertically uniform design objectives. Without such adjustments at $x = 1$ in the initial design, the isotherms extend from the top and touch the right wall $x = 1$ horizontally. Thus, the isotherms near the interface in the liquid get slanted and the vertical uniformities are lost.

The transient characteristics of the resultant flow field are different for the initial and optimal designs. In the initial design there is one major flow cell. The centre of this cell is towards the lower part of the liquid region and its $y$-position is decreasing as solidification progresses. For the inverse design solution, a secondary flow cell develops at the top right corner that pushes the centre of the major cell even lower. At later stages, the major cell breaks up into smaller and weaker ones until finally the convection has died out. The complicated heating/cooling conditions of the inverse design at $x = 1$ are responsible for the development of the above transient flow pattern.

5. CONCLUSIONS

In this work, an adjoint method formulation is presented for the inverse design of solidification processes with natural convection. The objective was to control the solidification process such that a desired interface location (thus growth velocity) and interface heat flux are achieved. In an example problem, the inverse design objectives were chosen to eliminate vertical non-uniformity in a directional solidification process of liquid aluminum confined in a square mold. The implementation of the optimization problem of the inverse formulation is carried out by the conjugate gradient method, while the direct, adjoint and sensitivity problems in each CGM iteration are solved by the finite element method. Through the direct problem solver, we also examined how accurately the inversely calculated heating/cooling boundary conditions can reproduce the desired interface data.

The current study has chosen relatively moderate convection strength ($Ra \sim 10^4$) with simple geometry settings, although the adjoint formulation itself does not rely on these choices. Further parameter studies and tests on more complicated cases remain to be done in the future to establish the robustness and convergence features of the present algorithms as well as to examine the convection strength limits to which the current algorithms are applicable. Modifications of the cost functional formulation to include regularization terms should also be considered to speed up convergence. In addition, other optimization techniques and preconditioning are currently examined. From the point of view of applications, work is being carried out to extend the presented methodology to an alloy solidification model and examine control problems related to morphological stability.

ACKNOWLEDGEMENTS

The results presented in this paper were obtained in the course of research sponsored by the National Science Foundation under a PYI award DDM-9157189 and a grant CTS-9115438 to Cornell University and with support from Alcoa Laboratories. The computing for this project was supported by the Cornell Theory Center, which receives major funding by the NSF and IBM.
Figure 11. Temperature and flow fields at times $t = 0.05$ and $0.12$ for the initial (left) and optimal (right) designs
Figure 12. Temperature and flow fields at times \( t = 0.22 \) and 0.32 for the initial (left) and optimal (right) designs.
Corporation, with additional support from the New York State. The authors gratefully acknowledge these contributions.

APPENDIX: DERIVATION OF THE ADJOINT EQUATIONS

Let $\mathcal{F}$ and $\mathcal{G}$ denote the sensitivity operators for the sensitivity thermal and fluid flow problems as are defined by the corresponding equations (31)–(38). The adjoint operators $\mathcal{F}^*$ and $\mathcal{G}^*$ are defined from the following Lagrange identities:15

\[
(\mathcal{F}^* \psi, \Theta)_{L^2(\omega(t) \times [0, t_{\text{max}}])} = (\psi, \mathcal{F}(\Theta))_{L^2(\omega(t) \times [0, t_{\text{max}}])} = 0 \quad (46)
\]

\[
(\mathcal{G}^* \phi, U)_{L^2(\omega(t) \times [0, t_{\text{max}}])} = (\phi, \mathcal{G}(U))_{L^2(\omega(t) \times [0, t_{\text{max}}])} = 0 \quad (47)
\]

where the definition of inner product: $(f, g)_{L^2(\omega(t) \times [0, t_{\text{max}}])} \equiv \int_0^{t_{\text{max}}} \int_{\omega(t)} f \cdot g \, d\Omega \, dt$ is used.

Let us first start from $(\phi, \mathcal{G}(U))_{L^2(\omega(t) \times [0, t_{\text{max}}])} \equiv 0$ to calculate $\mathcal{G}^*$, i.e.

\[
\int_0^{t_{\text{max}}} \int_{\omega(t)} \phi \cdot \left\{ \frac{\partial U}{\partial t} + (\nabla U) \mathbf{u} + (\nabla \mathbf{u}) \mathbf{U} + \nabla \Pi - Pr \nabla \cdot \nabla U + Pr Ra \Theta \mathbf{e}_g \right\} \, d\Omega \, dt = 0 \quad (48)
\]

The Reynolds formula for the continuously deforming domain $\omega(t)$, takes the following form:

\[
\frac{d}{dt} \int_{\omega(t)} A \, d\Omega = \int_{\partial \omega(t)} \frac{\partial A}{\partial t} \, d\Omega + \int_{\Gamma(t)} A v_t \cdot \mathbf{n} \, d\Gamma \quad (49)
\]

where $v_t$ and $\mathbf{n}$ are the boundary velocity and unit normal vector, respectively. The first term of equation (48) can now be written as follows:

\[
\int_0^{t_{\text{max}}} \int_{\omega(t)} \phi \cdot \frac{\partial U}{\partial t} \, d\Omega \, dt = \int_{\omega(t_{\text{max}})} \phi(x, t_{\text{max}}) \cdot U(x, t_{\text{max}}) \, d\Omega - \int_{\omega(0)} \phi(x, 0) \cdot U(x, 0) \, d\Omega - \int_0^{t_{\text{max}}} \int_{\omega(t)} \mathbf{U} \cdot \frac{\partial \phi}{\partial t} \, d\Omega \, dt + \int_0^{t_{\text{max}}} \int_{\Gamma(t)} \phi \cdot \mathbf{v}_t \cdot \mathbf{n} \, d\Gamma \, dt
\]

\[
= - \int_0^{t_{\text{max}}} \int_{\omega(t)} \mathbf{U} \cdot \frac{\partial \phi}{\partial t} \, d\Omega \, dt \quad (50)
\]

where we already introduced the zero final condition and non-slip bounday condition for the adjoint velocity $\phi$, i.e.

\[
\phi(x, t_{\text{max}}) = 0, \quad x \in \omega(t_{\text{max}}) \quad (51)
\]

\[
\phi(x, t) = 0, \quad x \in \Gamma(t) \quad (52)
\]

Integrating by parts each term on the left-hand side of equation (48) leads to the following equation:

\[
\int_0^{t_{\text{max}}} \int_{\omega(t)} \left\{ \mathbf{U} \cdot \left[ - \frac{\partial \phi}{\partial t} - (\nabla \phi) \mathbf{u} + (\nabla \mathbf{u})^T \phi + \nabla \pi - Pr \nabla^2 \phi \right] + Pr Ra (\phi \cdot \mathbf{e}_g) \Theta \right\} \, d\Omega \, dt = 0 \quad (53)
\]

where the adjoint pressure $\pi$ was already defined as

\[
\pi(x, t) = -\lambda \nabla \cdot \phi(x, t), \quad (x, t) \in \omega(t) \times [0, t_{\text{max}}] \quad (54)
\]
The above equation can be rearranged as follows:

\[
\int_0^{t_{\text{max}}} \int_{\Omega(t)} \mathbf{U} \cdot \left\{ -\frac{\partial \phi}{\partial t} - (\nabla \phi) \mathbf{u} + (\nabla \mathbf{u})^T \phi + \nabla \pi - Pr \nabla^2 \phi + Pr Ra \psi \nabla \theta \right\} \, d\Omega \, dt \\
+ \int_0^{t_{\text{max}}} \int_{\Omega(t)} Pr Ra(\phi \cdot \mathbf{e}_x \Theta - \psi \mathbf{U} \cdot \nabla \theta) \, d\Omega \, dt = 0
\] (55)

We can thus define the adjoint velocity operator \( G^* \) such that

\[
G^*(\phi) \equiv -\frac{\partial \phi}{\partial t} - (\nabla \phi) \mathbf{u} + (\nabla \mathbf{u})^T \phi + \nabla \pi - Pr \nabla^2 \phi + Pr Ra \psi \nabla \theta = 0
\] (56)

With the above definition of \( G^* \), equation (55) leads to the following relation between the two adjoint fields \( M \) and \( \psi \):

\[
\int_0^{t_{\text{max}}} \int_{\Omega(t)} \phi \cdot \mathbf{e}_x \Theta \, d\Omega \, dt = \int_0^{t_{\text{max}}} \int_{\Omega(t)} \psi \mathbf{U} \cdot \nabla \theta \, d\Omega \, dt
\] (57)

So far the adjoint velocity field \( \phi \) is defined as one that obeys equation (56), with the final condition of equation (51) and the boundary non-slip condition of equation (52).

The derivation of the operator \( F^* \) follows similar steps to those used to derive \( G^* \). We start from

\[
\int_0^{t_{\text{max}}} \int_{\Omega(t)} \psi \left( \frac{\partial \Theta}{\partial t} + \mathbf{u} \cdot \nabla \Theta + \mathbf{U} \cdot \nabla \theta - \nabla^2 \Theta \right) \, d\Omega \, dt = 0
\] (58)

Integration by parts of the first term of the above equation leads to the following:

\[
\int_0^{t_{\text{max}}} \int_{\Omega(t)} \psi \left( \frac{\partial \Theta}{\partial t} + \mathbf{u} \cdot \nabla \Theta + \mathbf{U} \cdot \nabla \theta - \nabla^2 \Theta \right) \, d\Omega \, dt = \int_0^{t_{\text{max}}} \int_{\Omega(t)} \psi \mathbf{U} \cdot \nabla \theta \, d\Omega \, dt + \int_0^{t_{\text{max}}} \int_{\Gamma_1} \psi \Theta(v_f \cdot \mathbf{n}) \, d\Gamma \, dt \\
+ \int_{\Omega(t)} \Theta(\mathbf{x}, t_{\text{max}}) \mathbf{v}(\mathbf{x}, t_{\text{max}}) \, d\Omega \, dt - \int_{\Omega(t)} \Theta(\mathbf{x}, 0) \mathbf{v}(\mathbf{x}, 0) \, d\Omega.
\] (59)

This can be simplified as

\[
\int_0^{t_{\text{max}}} \int_{\Omega(t)} \psi \left( \frac{\partial \Theta}{\partial t} + \mathbf{u} \cdot \nabla \Theta + \mathbf{U} \cdot \nabla \theta - \nabla^2 \Theta \right) \, d\Omega \, dt = \int_0^{t_{\text{max}}} \int_{\Omega(t)} \Theta \frac{\partial \psi}{\partial t} \, d\Omega \, dt + \int_0^{t_{\text{max}}} \int_{\Gamma_1} \psi \Theta(v_f \cdot \mathbf{n}) \, d\Gamma \, dt
\] (60)

after the following final condition for \( \psi \) was introduced:

\[
\psi(\mathbf{x}, t_{\text{max}}) = 0, \quad \mathbf{x} \in \Omega(\mathbf{r})
\] (61)

After integration by parts of every term in equation (58), we have the following:

\[
\int_0^{t_{\text{max}}} \int_{\Omega(t)} \Theta \left\{ -\frac{\partial \psi}{\partial t} - \mathbf{u} \cdot \nabla \psi - \nabla^2 \psi + \phi \cdot \mathbf{e}_x \right\} \, d\Omega \, dt \\
+ \int_0^{t_{\text{max}}} \int_{\Gamma_1} \Theta \left[ \frac{\partial \psi}{\partial n} - (v_f \cdot \mathbf{n}) \psi \right] \, d\Gamma \, dt - \int_0^{t_{\text{max}}} \int_{\Gamma_0} \psi \Delta q_0 \, d\Gamma \, dt
\] (62)
where we already used equation (57) and defined the following boundary conditions for $\psi$:

$$\frac{\partial \psi}{\partial n}(x, t) = 0, \quad (x, t) \in (\Gamma_0 \cup \Gamma_0') \times [0, t_{\text{max}}] \quad (63)$$

Let us further define the operator $\mathcal{F}^*$ as follows:

$$\mathcal{F}^*(\psi) \equiv -\frac{\partial \psi}{\partial t} - \mathbf{u} \cdot \nabla \psi - \nabla^2 \psi + \mathbf{f} \cdot \mathbf{e}_n = 0 \quad (64)$$

With the above definition and using equation (57), equation (62) takes the following form:

$$\int_0^{t_{\text{max}}} \int_{\Gamma_1} \Theta \left[ \frac{\partial \psi}{\partial n} - (\mathbf{v}_f \cdot \mathbf{n}) \psi \right] \, d\Gamma \, dt - \int_{\Gamma_{\text{in}}} \int_0^{t_{\text{max}}} \psi \Delta q_o \, d\Gamma \, dt = 0 \quad (65)$$

Let us define the last boundary condition for $\psi$ as follows:

$$\frac{\partial \psi}{\partial n}(x, t) = (\mathbf{v}_f \cdot \mathbf{n}) \psi + \theta_f(x, t) - \theta_m, \quad (x, t) \in \Gamma_1 \times [0, t_{\text{max}}] \quad (66)$$

Then equation (65) can be restated as follows:

$$\int_0^{t_{\text{max}}} \int_{\Gamma_1} \Theta(\theta_f - \theta_m) \, d\Gamma \, dt = \int_0^{t_{\text{max}}} \int_{\Gamma_{\text{in}}} \psi \Delta q_o \, d\Gamma \, dt \quad (67)$$

Comparing the above and equation (30), it implies that

$$S'(q_o(x, t)) = \psi(x, t; q_o), \quad (x, t) \in \Gamma_0 \times [0, t_{\text{max}}] \quad (68)$$

As such, the gradient of the cost functional is given by equation (68), where the adjoint field $\psi$ is defined via equations (61), (63), (64) and (66).

REFERENCES
