ADJOINT VARIABLE METHOD FOR THE THERMAL DESIGN OF EUTECTIC DIRECTIONAL SOLIDIFICATION PROCESSES IN AN OPEN-BOAT CONFIGURATION

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A computational method for the inverse design of a directional solidification process of a near-eutectic binary alloy driven by the coupled action of buoyancy, thermocapillary, and electromagnetic convection is presented. The objective is to calculate the mold cooling/heating conditions such that a stable desired interface growth with growth velocity $v_f$ and thermal gradient $G$ is achieved. The interface velocity $v_f$ and thermal gradient $G$ are chosen such that a diffusion-based growth is obtained in the presence of melt convection. Morphological stability is enforced by imposing an appropriate magnitude of $G/|v_f|$, which is determined a-priori based on the constitutional stability criterion. The design problem is posed as a functional optimization problem. The cost functional is defined so as to represent the deviation of the freezing interface thermal conditions from thermodynamic equilibrium. An appropriate continuum adjoint problem is defined such that an analytical expression for the gradient of the objective function is obtained. The conjugate gradient method coupled with the finite element solutions of the continuum direct, sensitivity, and adjoint problems is employed for solving the inverse problem. The method is demonstrated with an example of calculating the boundary thermal fluxes for the directional growth of an Sb-8.6% Ge melt in an open-boat configuration under the influence of an external horizontal magnetic field such that a stable vertical interface advances from left to right with a desired growth velocity.

INTRODUCTION

Optimal design or control problems involve selecting design/control variables for a system governed by partial differential equations (PDEs) to optimize a given design objective. Many of these problems can very often be posed as inverse problems in which, in addition to the various field equations, incomplete conditions are available on one part of the boundary, whereas over specified boundary conditions are supplied on another part of the boundary or inside the domain. These problems are ill-posed in the sense that their solution (if it exists) is unstable to perturbations.

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Examples of these inverse problems include aerodynamic duct design [1], drag reduction [2], parameter estimation [3], and many more.

In the context of thermal design problems, significant attention has been given to conduction-based inverse heat transfer problems [4, 5]. Some attention also has been given to inverse heat transfer problems involving natural or forced convection [6, 7, 8]. Applications to solidification process design also have been addressed in the past few years [9]. The emphasis of these papers is on the design and control
of mold cooling/heating conditions such that a desired solid–liquid interface morphology is achieved. Various algorithms and numerical techniques were developed to calculate the unknown functions. A particularly popular approach is the infinite-dimensional iterative regularization scheme [5], in which an appropriate continuum adjoint problem is defined that allows the analytical calculation of the gradient of the objective function.

In a recent article, Yang and Zabaras [10] posed and solved a design problem in the directional solidification of dilute binary alloys in a rectangular mold using the adjoint method. An extension of the methodology proposed in [10] to include the effects of an externally imposed magnetic field is presented in [11]. Application of magnetic fields has several advantages in the solidification system as, for example, damping of the flow and temperature oscillations [12, 13] in the melt and hence ensuring an improved crystal quality. In this work, we generalize the earlier analysis and techniques to the inverse design of directional solidification processes of eutectic binary alloys. In particular, we consider the directional solidification of an electrically conducting binary eutectic alloy in an open-boat configuration in which melt convection is driven by the combined action of buoyancy, thermocapillary, and electromagnetic forces. The motivation for considering this problem is twofold. First, the methods and design optimization techniques developed here can be easily extended to the design of open-boat Bridgman crystal growth processes for the production of semiconductor materials. Second, there is a never-growing interest in the processing of near-eutectic alloys because of their excellent high-temperature strength and mechanical properties. Mathematical methodologies for the design of eutectic solidification will thus help in the development of solidification processes that result in improved mechanical properties and microstructures for various eutectic alloys.

In this paper, we address the particular problem of designing mold wall thermal boundary conditions such that with coupled buoyancy, thermocapillary, and electromagnetic convection in the melt, a desired stable interface grow is achieved with front velocity $v_f$ and heat flux $G$. Control of the interfacial quantities $G$ and $v_f$ and ensuring stable interface growth are issues of tremendous importance in the eventual design of cast materials with desired mechanical properties. The interface morphological stability is enforced here by imposing an appropriate magnitude of $G/|v_f|$, which is determined a-priori based on the constitutional stability criterion. Several more advanced stability criteria that include interfacial–tension effects, melt flow, crystalline anisotropy, and so on, have been proposed in recent years. However, for the purpose of the present inverse design problem, we will consider that the absence of constitutional undercooling is sufficient for the existence of a stable growth. The interested reader is advised to consult [14, 15] for a comprehensive review of morphological stability in solidification systems.

The structure of this article is as follows. The next section presents the direct model definition for a binary eutectic alloy solidification process in an open-boat configuration in the presence of an external magnetic field. This section also defines a reference directional solidification problem that violates the a priori assumption of stability and exhibits macroscopic interface curvature because of melt convection. In the following section, we present a precise definition of the inverse design eutectic solidification problem incorporating the coupled effects of thermocapillary,
buoyancy, and electromagnetic convection in the melt. This inverse problem leads to two separable subproblems, one in the solid phase and another in the melt. This article focuses only on the inverse problem in the melt phase as the inverse problem in the solid domain is a standard inverse heat conduction problem (IHCP) and is addressed in earlier works. The inverse problem in the melt domain is a new inverse problem not addressed earlier in the literature. In this article, we propose an optimal design technique to solve the above inverse problem, which couples a conjugate gradient method (GM) with gradients computed using the adjoint equation approach with appropriate regularization to ensure well-posedness. We refer to this combined adjoint/CGM algorithm as the adjoint variable method (AVM). The details of this methodology are addressed in that section. In the final two sections, we demonstrate and validate the developed method with an example of designing the boundary heat fluxes for the directional solidification of a near-eutectic antimony-germanium binary alloy in an open-boat configuration with an imposed magnetic field such that growth proceeds with a stable solid–liquid interface with interface velocity $v_f$ and heat flux $G$.

**DIRECT BINARY ALLOY SOLIDIFICATION PROBLEM WITH COUPLED THERMOCAPILLARY, BUOYANCY, AND ELECTROMAGNETIC CONVECTION IN THE MELT**

Here, we restrict attention to a binary eutectic alloy. The composition of the alloy is defined by a continuous scale between its two end members A and B. The solidification behavior of the alloy depends on which side of the eutectic composition, $C_E$, the alloy composition, $C$, lies, and hence the phase diagram has two branches, which correspond to alloys of subeutectic composition ($C_A < C < C_E$) and supereutectic composition ($C_E < C < C_B$), respectively. Fluid of eutectic composition ($C = C_E$) behaves as a pure melt, crystallizing to form a solid of eutectic composition.

Assuming that solidification is occurring under conditions of thermodynamic equilibrium, the temperature and composition of the fluid adjacent to the solidification front are constrained to lie on the appropriate branch of the liquidus curve. Given the interfacial temperature, the composition of the solid produced is then determined by the corresponding branch (subeutectic or supereutectic) of the solidus curve. For alloy compositions $C$ such that $C \neq C_E$, the preferential solidification of one or the other phase (i.e., $\alpha$ or $\beta$ phases) results in rejection of solute such that there is a gradual evolution of the mean composition of the residual melt toward the eutectic composition as crystallization proceeds. Complete solidification of a binary eutectic alloy can only occur if it is cooled below its eutectic temperature.

In this article, we adopt the limiting “sharp-interface” approximation. In this approximation, the interface is treated as locally flat with a sharp interface between the solid and fluid. The mushy layer is formally enforced to have infinitesimal thickness with the interfacial fluid having a composition and temperature corresponding to the eutectic. However, the bulk composition of the solid formed need not be eutectic because of the presence of the thin mushy layer and is instead controlled by mass transfer within the fluid.
The particular model was selected for two reasons. At first, the sharp-interface model is mathematically and fluid dynamically easier to treat, while at the same time capturing the essential physics (see [16] for corroboration of model predictions with experiments for several aqueous solution binary eutectic systems). Second, in this work we propose design optimization methods to control the solidification process such that growth occurs under stable conditions. The sharp-interface model is the most appropriate and accurate model for the description of such stable growth systems.

**Mathematical Model**

Consider the directional solidification of an incompressible, electrically conducting binary eutectic alloy in a two-dimensional rectangular box with an open boundary under the influence of an external magnetic field \( B_0 \) (see Figure 1). At time \( t = 0^+ \), a cooling heat flux is applied on the mold boundary \( \Gamma_{os} \) and solidification commences. The resulting convection in the melt is determined by the combined action of buoyancy, surface tension, and electromagnetic forces. Motion in the presence of a magnetic field gives rise to a Lorentz force [17], which acts on the fluid and appears as an additional body force in the momentum equations.

The equations governing the binary alloy solidification system are now introduced. The basic equations used in the simulation of the melt flow are the incompressible Navier–Stokes equations, including the Lorentz body force term. The Boussinesq approximation is used for defining the effects of buoyancy. The other main equations governing the fluid flow in the liquid domain are the energy equation and solute transport equation. In dimensionless form (see the Nomenclature section for the definition of the various dimensionless fields), these equations are written as follows:

\[
\nabla \cdot \mathbf{v} = 0, \quad (1)
\]

\[
\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \Pr \nabla^2 \mathbf{v} - \frac{R_a T \Pr \theta_l - R_a c \Pr c}{\varepsilon} \mathbf{e}_g + \frac{H a^2 \Pr [\mathbf{v} \times \mathbf{e}_B] \times \mathbf{e}_B}{\nabla}, \quad (2)
\]

\[
\frac{\partial \theta_l}{\partial t} + \mathbf{v} \cdot \nabla \theta_l = \nabla^2 \theta_l \quad (3)
\]

\[
\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \Le^{-1} \nabla^2 c \quad (4)
\]

Heat transfer in the solid is by conduction and is written in dimensionless form as

\[
\frac{\partial \theta_s}{\partial t} = R_x \nabla^2 \theta_s, \quad (5)
\]

where \( R_x \equiv \frac{x_s}{x_l} \) is the ratio of the thermal diffusivities of the solid and the melt.

The interfacial temperature of the liquid and solid and composition of the liquid are given by

\[
\theta_l = \theta_s = \theta_E \quad \text{and} \quad c = c_E \quad \text{on} \quad \Gamma_I(t) \quad (6)
\]
The solid composition is determined by the rate at which composition is transported diffusively to and from the solidification front, and is given by the dimensionless mass balance

\[ (c_s - c_E)(v_f \cdot n) = \text{Le}^{-1} \frac{\partial c}{\partial n} \]  

where the normal vector \( n \) is pointing out from the liquid domain.

In addition to the mass balance, we also have a thermal balance, in which the heat supplied by the fluid and the latent heat released upon crystallization of fresh solid are balanced by the conductive transport of heat into the solid, i.e.,

\[ R_k \frac{\partial \theta_s}{\partial n} - \frac{\partial \theta_l}{\partial n} = \text{Ste}^{-1}(v_f \cdot n) \]  

Initially, the fluid has uniform temperature \( \theta_l = \theta_i \), composition \( c_l = c_i \), and is motionless \( (v = 0) \). On the solid–liquid interface \( \Gamma_{il}(t) \) and the bottom and outer liquid boundaries \( (\Gamma_{bl}(t) \cup \Gamma_{ol}(t)) \), we apply the no-normal-flow and no-slip conditions \( v = 0 \). The surface tension on the free surface \( \Gamma_{ul}(t) \) is approximated by a linear function of temperature and is given by

\[ \sigma(T) = \sigma_0 \left[ 1 - \gamma_T(T - T_o) + O(T - T_o)^2 \right] \]

where \( \gamma_T = -(1/\sigma_o)(\partial \sigma / \partial T) \). In this work, solutal-capillary effects are neglected because of the high magnitude of the Lewis number \( (\text{Le} = 319.0) \) of the system, which limits solutal-capillary effects to regions very close to the solid–liquid interface, where advection is suppressed. The tendency of thermocapillary effects to be favored by large Lewis numbers was also addressed in [18] and [19].

The hydrodynamic boundary condition on the free surface \( \Gamma_{ul} \) reflects the effects of the varying surface tension because of temperature variation on the free

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**Figure 1.** Schematic of the binary alloy solidification problem in an open-boat configuration under the influence of an externally applied magnetic field.
where \( \mathbf{t} \) is an independent tangent vector to the free surface. This boundary condition appears as a flux (Neumann) boundary condition in the solution of the flow equations once the temperature equation has been solved. Note that the free-surface deformation is neglected and a no-penetration boundary condition is imposed on the free surface. Finally note that, because the temperature of the solid–liquid interface is constrained to be equal to the eutectic temperature, the rate of solidification is not directly influenced by the diffusion of mass, but is defined by the heat balance alone.

It is assumed that adiabatic conditions are maintained on \( \Gamma_{hl} \cup \Gamma_{il} \). The equilibrium condition (see Eq. (6)) on the interface imposes a Dirichlet boundary condition on \( \Gamma_I \). A problem dependent flux/temperature condition on the outer liquid boundary \( \Gamma_{ol} \) completes the definition of the thermal problem defined on \( \Omega_l \). The solutal boundary conditions are provided by the impermeable wall condition on the outer boundaries and a Dirichlet condition on the interface \( \Gamma_I \) (see Eq. (6)).

In the solid phase \( \Omega_s \), the equilibrium condition (Eq. (6)) on the interface \( \Gamma_I \), the problem-dependent flux/temperature condition on \( \Gamma_{os} \), and the adiabatic conditions on the top and bottom solid boundaries (\( \Gamma_{ts} \cup \Gamma_{bs} \)) provide the required boundary conditions for the solution of the heat transport problem.

Finally, note that the solidification front is typically macroscopically curved because of transport of heat by both thermal and compositional convection in the fluid. The resulting shape and position of the solid–liquid interface are determined only through the solution of the nonlinear transport equations and constitute an integral part of the solution of the solidification problem.

**Solution Procedure**

A stabilized SUPG/PSPG formulation using an equal-order-velocity-pressure interpolation as proposed by Tezduyar et al. [20, 21] is implemented in this work for the fluid flow simulation. In this method, stabilization is achieved by adding two terms to the standard Galerkin formulation of the problem. The first term leads to the popular SUPG formulation, which has been applied quite successfully to both incompressible and compressible flow problems for more than a decade. It prevents the oscillations caused by the presence of advection terms without introducing excessive numerical dissipation. The second stabilization term is the PSPG term, which was introduced in [20, 21] to accommodate equal-order-interpolation velocity pressure elements. In this work, the above formulation for the simulation of incompressible flows has been modified to account for additional contributions from buoyancy, electromagnetic, and thermocapillary forces. This formulation for the fluid flow problem is combined with a standard SUPG formulation for the heat and solute transport equations with discontinuous contributions from buoyancy, electromagnetic, and thermocapillary forces. This formulation for the fluid flow problem is combined with a standard SUPG formulation for the heat and solute transport equations with discontinuous contributions from buoyancy, electromagnetic, and thermocapillary forces. The above formulations are coupled with a moving/deforming finite element method (FEM) procedure [33] to allow explicit tracking of the moving solid–liquid interface. The methodology involves defining separate finite element grids for the solid and melt domains at the initial time and dynamically deforming the grids at subsequent
times based on the freezing interface velocity. The position and velocity of the moving solid–liquid interface is determined via the solution of the Stefan condition using an energy preserving formulation [33]. A predictor–multicorrector scheme is used for the time integration of the heat and solute transport equations, while a T1 formulation [20] is used for the temporal advancement of the flow equations. The solution of the various subproblems is achieved using a decoupled solution scheme at a given time step. Our experience with solidification simulations has shown that such an approach is quite accurate as well as computationally effective. An LU-factorized preconditioner coupled with a biconjugate gradient stabilized Bi-CGSTAB method [22] along with mass lumping has been used in the linear system solvers to improve the computational performance of the various algorithms.

The formulation and numerical solution procedures have been verified successfully through comparisons with reported numerical results for the solidification of a pure substance [23]. The numerical accuracy and fidelity of the flow solver also has been confirmed through extensive comparisons with existing numerical solutions for several benchmark incompressible flow problems as well as existing numerical solutions for coupled thermocapillary and buoyancy-driven flow in a rectangular cavity [24, 25, 26]. The additional influence of an externally applied magnetic field also has been numerically studied and compared with reported results [26].

**Reference Binary Eutectic Alloy Solidification Problem**

Consider a cavity with an open free surface of dimensions 20 mm × 20 mm filled with molten Sb-8.6 wt% Ge, initially at 100°C above the eutectic temperature (592°C). At time \( t = 0^+ \), the left wall \( \Gamma_{os} \) is suddenly cooled to a temperature 100°C below the eutectic temperature and maintained at that temperature for times \( t > 0 \). All other walls are insulated. The thermophysical properties of this system are listed in Table 1. The binary phase diagram corresponding to this system is shown in Figure 2. The thermophysical properties were compiled from various sources, including [13], [27], and [28]. The resulting dimensionless quantities are listed in Table 2. The reasons for the choice of this particular semiconductor melt system for the current study are the following:

- The assumptions of the model restrict the applicability of the developed methods to systems that are electrically conducting at their neutral state, such as metallic and semiconductor melts, and this eliminates the choice of the relatively well studied aqueous salt solution systems (e.g. \( \text{NH}_4\text{Cl}, \text{Na}_2\text{CO}_3, \text{Na}_2\text{SO}_4, \text{K}_2\text{CO}_3 \), etc.).
- For metallic systems such as, for example, Pb–Sn, where the Lewis number is extremely high (\( \approx 10^4 \)), the solutal boundary layer is extremely thin and concentration gradients are very high close to the interface, and, hence, it is extremely difficult to achieve a stable interface growth for such systems through thermal boundary control under practical growth conditions.

The above physical arguments restrict the applicability of the methodology presented here to electrically conducting binary eutectic alloy melts with moderate and low Lewis numbers (\( \mathcal{O}(10^2–10^3) \)).
At $t = 0^+$ the freezing process starts and takes place under standard laboratory conditions (normal gravity and zero magnetic field). We refer to this problem as the \textit{reference design problem}. A moderate FE mesh of 960 bilinear elements was used in the solid domain and 1500 elements in the liquid domain. It is realized that this grid system might not be adequate to resolve all the details of the double-diffusive flow structures in the liquid region as well as the strong thermocapillary corner flow near the solid–liquid interface. The selected mesh size is such that the bulk flow

\begin{table}
\centering
\caption{Physical constants for the Sb-8.6\% Ge system}
\begin{tabular}{l l l}
\hline
Symbol & Value \\
\hline
Density of the melt & $\rho_l$ (kg/m$^3$) & 6697.0 \\
Density of the solid & $\rho_s$ (kg/m$^3$) & 6697.0 \\
Viscosity of the melt & $\mu$ (Ns/m$^2$) & $2.0 \times 10^{-3}$ \\
Thermal expansion coefficient & $\beta_T$ (°C$^{-1}$) & $1.1 \times 10^{-4}$ \\
Solutal expansion coefficient & $\beta_c$ (wt\%°C$^{-1}$) & $3.5 \times 10^{-3}$ \\
Electrical conductivity & $\sigma_e$ (A/Vm) & $2.7 \times 10^6$ \\
Diffusivity & $D$ (cm$^2$/s) & $5.4 \times 10^{-4}$ \\
Thermal conductivity of the solid & $k_s$ (W/mK) & 25.9 \\
Thermal conductivity of the melt & $k_l$ (W/mK) & 22.0 \\
Solid specific heat & $c_s$ (kJ/kgK) & 0.207 \\
Liquid specific heat & $c_l$ (kJ/kgK) & 0.21 \\
Latent heat & $L$ (kJ/kg) & 163.17 \\
Linear thermal coefficient of surface tension & $\partial\sigma/\partial T$ (dyn/cmK) & $-0.07$ \\
\hline
\end{tabular}
\end{table}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{Figure2}
\caption{Equilibrium phase diagram of the Sb–Ge system.}
\end{figure}
structures and overall transport patterns are captured sufficiently. Because of the extreme computational cost associated with inverse simulations (in comparison with standard direct simulations), the selected mesh size should only be viewed as a compromise between accuracy and computational cost associated with such simulations. An initial dimensionless time step of $\Delta \tau = 10^{-4}$ was utilized for the first 200 steps to ensure stable solutions during this rapid transient, after which a constant time step of $\Delta \tau = 0.001$ was used. For a total simulation time of $\tau = 1.5$, the calculations required approximately 6000 CPU seconds on an Intel Pentium III, 500 MHz node of the AC3 velocity cluster provided by the Cornell Theory Center (CTC).

For illustration, the convective flow field and fluid composition corresponding to a few intermediate stages of the solidification process are presented in Figure 3. After the thermally dominated initial transient has passed (at which time the fluid has essentially lost all superheat), the compositionally heavy fluid settles at the bottom (see Figure 3h) and slowly forms a stratified layer. This layer continues to grow until the entire fluid composition evolves toward the eutectic at all levels (see Figure 3i). This process, termed laminar box filling, has been studied both theoretically and experimentally [29]. The flow reversal observed in the bottom-right-hand corner of Figure 3c is a typical feature of natural convection in a stratified fluid [29]. The composition of the solid product shown in Figure 4a reflects the evolution of the fluid flow and composition fields. Note the complex vertical variation in the solute composition because of the melt flow.

Considering all the computed continuum fields, we are particularly interested in determining if the a priori assumption of a stable sharp-interface growth does in fact hold well. This is particularly important considering the fact that in many solidification systems the interface is typically unstable, leading to the formation of a dendritic microstructure. Figure 4b shows the dimensionless contours of the quantity $\Delta \equiv G/|v_f| + m(C_E - C_o)/D_L$ as a function of the interface y-coordinate and time (here $G$ and $v_f$ are obtained as part of the solution to the reference design problem). Based on the constitutional stability criterion, this quantity has to be nonnegative to ensure stable growth (refer to the discussion in the enforcement of the constitutional stability condition section). However, as can be seen from Figure 4b, it is clear that the stability condition is only satisfied during the early

| Table 2. Dimensionless groups and their characteristic values |

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pr</td>
<td>0.017</td>
</tr>
<tr>
<td>$m$</td>
<td>$-0.02525$</td>
</tr>
<tr>
<td>Ste</td>
<td>0.1348</td>
</tr>
<tr>
<td>Ha</td>
<td>36.74 (0.05 T)</td>
</tr>
<tr>
<td>$R_k$</td>
<td>1.177</td>
</tr>
<tr>
<td>$R_z$</td>
<td>1.2512</td>
</tr>
<tr>
<td>$Ra_c$</td>
<td>$6.275 \times 10^4$</td>
</tr>
<tr>
<td>$Ra_T$</td>
<td>$1.644 \times 10^5$</td>
</tr>
<tr>
<td>$Ma_T$</td>
<td>$-3982.02$</td>
</tr>
<tr>
<td>Le</td>
<td>319.0</td>
</tr>
</tbody>
</table>
stages of solidification. Clearly, the calculated solution after the onset of instability is not physical. The reason for the onset of such an instability lies mainly in the fact that the rejected solute near the advancing solid–liquid interface cannot be diffused sufficiently rapidly (because of $D_l \ll \alpha_f$), which leads to a constitutionally supercooled liquid ahead of the solidification front. Such a "constitutional supercooling" leads to the formation of a variety of microscopically complicated microstructures (cells, dendrites), resulting in a significant depreciation in the quality of the final crystal. In the following section, we address the issue of designing the thermal boundary

Figure 3. Contours of the fluid stream function (a)–(c) isotherms (d)–(f), and iso compos (g)–(i) for the reference eutectic solidification simulation. Simulation results are shown at dimensionless times $\tau = 0.1$, $\tau = 0.8$, and $\tau = 1.5$. Note that clockwise circulations are denoted by dashed lines, whereas counterclockwise recirculating cells are depicted by solid lines.
Figure 4. (a) Contour plot of the solid composition (in wt% germanium) for the reference solidification problem; (b) examination of the constitutional stability assumption at the solid–liquid interface for the reference design problem. Dimensionless contours of $\Delta = G/|v| + m(C_E - C_o)/D_L$ are displayed. Note that stable growth ($\Delta \geq 0$) is achieved only for a very short period during the entire solidification process.
conditions for this reference problem so as to achieve a desired flux $G$ and growth velocity $v_f$ on the interface while at the same time ensuring a stable interface growth. To facilitate the objectives of achieving diffusion-based growth conditions, we subject the solidification system to a strong external magnetic field of strength 0.05 T ($H_a = 36.74$). The application of this strong external magnetic field supplements the optimal thermal boundary fluxes in achieving the design intent through the damping of melt flow.

**DEFINITION OF THE INVERSE ALLOY SOLIDIFICATION PROBLEM**

Referring to the above reference design problem, we pose the following inverse problem to achieve the design objectives of a desired stable solid–liquid interface with interfacial flux $G$ and velocity $v_f$:

Find the cooling heat flux $q_{os}(x, t)$ on the boundary $\Gamma_{os}$ as well as the heat flux condition $q_{ol}(x, t)$ on the vertical mold wall $\Gamma_{ol}$ (see Figure 5a) so that in the presence of coupled thermocapillary, buoyancy, and electromagnetically driven convection in the melt, a desired flat-interface growth (with desired flux $G$ and growth velocity $v_f$) is achieved that is ensured to be morphologically stable.

The above inverse design problem can be divided into two subproblems, one inverse problem in the solid region and another in the liquid region. This is possible because, as part of the design objectives, the location of the interface $\Gamma_I$ is explicitly known through the given growth velocity $v_f$. Neglecting Joule heating, the inverse problem in the solid domain is the well-studied IHCP. The inverse problem in the liquid domain is a new inverse problem that has not been addressed in the literature and is depicted in Figure 5b. This inverse problem involves coupled effects of thermocapillary, buoyancy, and electromagnetic forces.

As a first step, in this work the *constitutional stability criterion* is considered to enforce the morphological stability of the solid–liquid interface. Details of this formulation are reviewed in the following section, along with some comments on the limitations of the proposed procedure.

**Enforcement of the Constitutional Stability Condition**

The general problem of morphological instability of the crystal melt interface in eutectic solidification is, in some ways, analogous to that of solidification of single-phase alloys. If the interface can be maintained stable in the plane-front configuration, eutectic or eutectic-like structures are obtained. When the interface breaks down, cellular and dendritic structures are obtained. However, there are also some fundamental differences in the instability phenomena, particularly the interface breakdown process. Unlike single phase alloys, binary eutectics can undergo two types of morphological instability—single phase or two phase. The latter is analogous to the morphological instability of a planar single-phase interface. During off-eutectic growth of a binary alloy, single-phase instability can occur and result in the appearance of mixed structures, that is, dendritic structures of one phase and interdendritic two-phase eutectic. The reason for this effect is that, because
of the long-range boundary layer built up ahead of the solid–liquid interface, one phase becomes heavily constitutionally undercooled.

In this article, in contrast to the above microstructural understanding of the instability phenomena, we take a macroscopic viewpoint of the interface breakdown process and restrict our discussion to the simple constitutional stability criterion. In particular, we consider the following constraint on the $G / |v_f|$ ratio:

$$
\frac{G}{|v_f|} = \frac{m_L (C_E - C_o)}{D_L}
$$

(11)

to be sufficient to ensure stability of the solid–liquid interface. Note that all the quantities shown in the above equation are in dimensional form. This condition prescribes a lower limit for the ratio $G / |v_f|$, above which the interface is ensured to be constitutionally stable. Experimental evidence reported in [31] shows that for compositions close to the eutectic, this estimate is actually a conservative one, in which case very low values of $G / |v_f|$ are sufficient to ensure stability of the advancing interface. The reason for this anomalous behavior is that, unlike single-phase solidification where solute mainly diffuses along a direction perpendicular to the solidifying front, in eutectic growth, the bulk of solute transport occurs along the solid–liquid interface (i.e., between the $\alpha$ and $\beta$ lamellae). This lateral solute transport decreases the solute buildup ahead of the solid–liquid interface, rendering the solid–liquid interface stable at even low values of $G / |v_f|$. These experiments also confirmed that eutectic-like structures are obtained with sufficiently high values of $G / |v_f|$ even in compositions sufficiently removed from the eutectic.

Based on the results of these experimental/theoretical studies, in this article, we enforce stability in the inverse simulations by explicitly choosing an interface.
thermal gradient $G$ and growth velocity $v_f$ such that $G/v_f$ marginally satisfies the constraint given in Eq. (11). For the slightly off-eutectics system considered in this article, this condition should suffice to ensure stable growth throughout the solidification process.

**Adjoint Variable Method**

In the following discussion, we present the essential algorithmic details of the adjoint method proposed to solve the above-described inverse design eutectic solidification problem.

**Definition of the optimization problem.** It is assumed that there is enough regularity of the boundary to allow us to work in the framework of $H^1(\Omega)$ functions. To ease the presentation of the various inner products and norms of functions $f$ and $g$, the following inner product notation is used in the rest of the paper:

$$ (f, g)_{\mathcal{D}} = \int_0^{t_{\text{max}}} \int_{\mathcal{D}} f \cdot g \; d\mathcal{D} \; dt, \quad \forall \; f, g \in L_2(\mathcal{D} \times [0, t_{\text{max}}]) $$

where we have used dot-product notation for the scalar product of vector functions or simple multiplication in the case of scalar functions and $\mathcal{D}$ refers to the domain over which the functions $f$ and $g$ are defined.

The space of admissible controls $\mathcal{U}$ is next defined as the Hilbert space $\mathcal{U} = H^1(\Gamma_{ol} \times [0, t_{\text{max}}])$. This space is such that the function as well as its derivatives are square integrable. The choice of such a design function space is dictated by the $H^1$ regularization introduced later in this article to ensure stability of the numerical algorithm. The inverse design problem in the melt can now be posed as a spatio-temporal optimization problem. With a guessed heat flux $q_{ol}(x, t), (x, t) \in \Gamma_{ol} \times [0, t_{\text{max}}]$, one can define a direct coupled thermocapillary-buoyancy-electromagnetic convection problem on the prescribed domain $\Omega(t)$. Let us denote its solution for the temperature, concentration, and flow fields as $\theta(x, t; q_{ol}), c(x, t; q_{ol})$, and $v(x, t; q_{ol})$, respectively. The equilibrium condition $\theta(x, t) = \theta_E(x, t) \in \Gamma_{I} \times [0, t_{\text{max}}]$ is not used in this direct problem definition, thus it is not guaranteed to be satisfied. For an arbitrary $q_{ol} \in H^1(\Gamma_{ol} \times [0, t_{\text{max}}])$, we define a cost functional:

$$ J(q_{ol}) = \frac{1}{2} \left[ \| \theta(x, t; q_{ol}) - \theta_E \|^2_{L_2(\Gamma_{I} \times [0, t_{\text{max}}])} \right] $$

$$ + \frac{\gamma}{2} \left[ \| q_{ol} \|^2_{L_2(\Gamma_{ol} \times [0, t_{\text{max}}])} + \| \nabla q_{ol} \|^2_{L_2(\Gamma_{ol} \times [0, t_{\text{max}}])} \right], $$

where $\gamma \in \mathbb{R}^+$ is an appropriate regularization parameter chosen based on the numerical errors in the algorithm. The two terms involving the heat flux $q_{ol}$ and its spatial derivative are introduced to ensure a stable numerical solution. The ill-posed nature of this kind of inverse problems, coupled with the severe numerical errors close to the singular corner region early in the considered solidification system, has necessitated the use of the present $H^1$-type regularization.
In this article, our objective is to construct a minimizing sequence 
\( q^k_{ol}(x, t) \in \mathcal{U}, \ k = 1, 2, \ldots \), that converges to at least a local minimum of \( \mathcal{J}(q_{ol}) \). If such a minimum can lead to an interface growth that is close enough to the desired thermodynamically consistent growth according to a certain accuracy measure and is constitutionally stable, then an acceptable design solution has been obtained.

To perform the optimization procedure that minimizes \( \mathcal{J}(q_{ol}) \in \mathcal{U} \), we will need to define a continuum sensitivity problem in terms of the sensitivity velocity field \( \mathbf{V}(x, t; q_{ol}) \), sensitivity temperature field \( \Theta(x, t; q_{ol}) \), and sensitivity concentration field \( C(x, t; q_{ol}) \). This linear problem (similar in form to the direct problem) is derived by computing the linear perturbations of the fields \( \theta(x, t; q_{ol}), c(x, t; q_{ol}), \) and \( \mathbf{v}(x, t; q_{ol}) \), respectively, with respect to the variations \( \Delta q_{ol}(x, t) \) of the design heat flux \( q_{ol} \). For the sake of brevity, we do not present the details of derivation of this system of equations in this article and advise the interested reader to consult [32] for a similar derivation. To realize the minimization of \( \mathcal{J}(q_{ol}) \), it is essential to find its gradient (or design derivative) \( \mathcal{J}'(q_{ol}) \) with respect to the design flux \( q_{ol} \).

After some tedious calculations (see [33]) an associated adjoint problem (see Box I) can be defined in terms of the adjoint velocity field \( \mathbf{\tilde{v}}(x, t; q_{ol}) \), adjoint temperature field \( \mathbf{\tilde{\Theta}}(x, t; q_{ol}) \) and adjoint concentration field \( \mathbf{\tilde{C}}(x, t; q_{ol}) \). Based on this adjoint problem derivation, we can show that the gradient of \( \mathcal{J}(q_{ol}) \) with respect to the scalar product \( (\cdot, \cdot)_{H^1(\Omega_{ol} \times [0,t_{\max}])} \equiv (\nabla \cdot, \nabla \cdot)_{L^2(\Gamma_{ol} \times [0,t_{\max}])} \) is given by

\[
\mathcal{J}'(q_{ol}) = z + \gamma q_{ol} \tag{14}
\]

In the above equation, \( z(x, t) \) is obtained by first calculating the solution component \( \mathbf{\tilde{v}}(x, t; q_{ol}) \) of the adjoint equations listed in Box I, followed by the solution of an additional variational equation on \( \Gamma_{ol} \):

\[
-\Delta z(x, t) + z(x, t) = \mathbf{\tilde{v}}(x, t; q_{ol}) \tag{15}
\]

In the solution of the above variational equation, Neumann boundary conditions are applied on \( \partial \Gamma_{ol} \) (boundary of \( \Gamma_{ol} \)).

Finally, it is essential to point out here that the derivation of the adjoint equations and entire inverse formulation presented in this article is strictly applicable to the two-dimensional case. The difficulty in extending the derivation to three dimensions lies basically in the nontrivial coupling between the flow fields and the electric potential fields in the three-dimensional case. This additional term in the flow equations and the fact that the no-slip condition fails to hold on the free surface introduces additional complexity in extending the present formulation to three dimensions. As yet, it is not clear how this problem can be circumvented to make the present formulation dimension independent.

**Conjugate gradient algorithm.** After having obtained an analytical expression for the exact gradient, any of the standard functional minimization techniques can be used for solving the above-defined optimization problem. Here, we shall use the nonlinear CGM for the optimization loop. The reason for selecting this type of gradient algorithm is its excellent “viscous” properties [5] while nearing the optimal point. The CGM constructs a sequence: \( q^0_{ol}, q^1_{ol}, \ldots, q^k_{ol}, \ldots \), to approach the optimum solution \( q_{ol} \) [34]. The optimization procedure is shown in Box II. Note
that, because of the choice of the $H^1$ function space for the control variable $q_{ol}$, all the norms and gradients within the CGM algorithm shown in Box II are also consistently defined in the same space.

The solution of the adjoint and sensitivity problems is numerically realized using a moving FEM in a way similar to the direct problem. The entire system of direct, adjoint, and sensitivity problems described here is implemented using an object-oriented approach. The presentation of these techniques is beyond the objectives of this article. More details on the application of object-oriented techniques to adjoint-based inverse design problems can be found in [35] and references therein.
Step I: Make an initial guess of \( q_{ol}^0 \in H^1(\Gamma_{ol} \times [0, t_{max}]) \), calculate \( \nabla q_{ol}^0 \), and set \( k = 0 \).

Step II. Calculate the conjugate search direction \( p^k(\mathbf{x}, t), (\mathbf{x}, t) \in \Gamma_{ol} \times [0, t_{max}] \):
1. Solve the coupled direct problem for \( \theta(\mathbf{x}, t; q_{ol}^k), \mathbf{v}(\mathbf{x}, t; q_{ol}^k), \) and \( c(\mathbf{x}, t; q_{ol}^k) \).
2. Evaluate \( \mathcal{J}(q_{ol}^k) \) from Eq. (13); if \( \mathcal{J}(q_{ol}^k) < \) tolerance, set \( \bar{q}_{ol}^k = q_{ol}^k \) and stop.
3. Solve the coupled adjoint problem backward in time for \( \psi(\mathbf{x}, t; q_{ol}^k), \tilde{\phi}(\mathbf{x}, t; q_{ol}^k), \) and \( \tilde{\rho}(\mathbf{x}, t; q_{ol}^k) \).
4. Solve Eq. (15) for \( z(\mathbf{x}, t; q_{ol}^k) \) for \( (\mathbf{x}, t) \in \Gamma_{ol} \times [0, t_{max}] \) and calculate \( \nabla z(\mathbf{x}, t; q_{ol}^k) \).
5. Set \( \mathcal{J}'(q_{ol}^k) = z(\mathbf{x}, t; q_{ol}^k) + \gamma q_{ol}^k \) for \( (\mathbf{x}, t) \in \Gamma_{ol} \times [0, t_{max}] \) and calculate \( \nabla \mathcal{J}'(q_{ol}^k) \).
6. Set \( \gamma^k = 0, \) if \( k = 0; \) otherwise,
\[
\gamma^k = \frac{\mathcal{J}'(q_{ol}^k)}{\nabla \mathcal{J}'(q_{ol}^k)}.
\]
7. Define \( p^k(\mathbf{x}, t) \): If \( k = 0, \) \( p^0 = -\mathcal{J}'(q_{ol}^k), \) \( \nabla p^0 = -\nabla \mathcal{J}'(q_{ol}^k); \)
\[
p^k = -\mathcal{J}'(q_{ol}^k) + \gamma^k p^{k-1},
\]
otherwise:
\[
\nabla p^k = -\nabla \mathcal{J}'(q_{ol}^k) + \gamma^k \nabla p^{k-1}.
\]

Step III: Calculate the optimal step size \( \varepsilon^k \):
1. Solve the coupled sensitivity problem for \( \hat{\Theta}(\mathbf{x}, t; q_{ol}^k, p^k), \hat{\mathbf{v}}(\mathbf{x}, t; q_{ol}^k, p^k), \) and \( \hat{C}(\mathbf{x}, t; q_{ol}^k, p^k) \).
2. Calculate \( \varepsilon^k \):
\[
\varepsilon^k = \frac{-[\mathcal{J}'(q_{ol}^k), p^k]_{L_2(\Gamma_{h0} \times [0, t_{max}])} + \gamma(q_{ol}^k, p^k)_{H^1(\Gamma_{h0} \times [0, t_{max}])}}{\nabla \hat{\Theta}(\mathbf{x}, t; q_{ol}^k, p^k)_{L_2(\Gamma_{h0} \times [0, t_{max}])} + \gamma \nabla p^k_{H^1(\Gamma_{h0} \times [0, t_{max}])}}.
\]

Step IV: Update \( q_{ol}^{k+1}(\mathbf{x}, t) = q_{ol}^k(\mathbf{x}, t) + \varepsilon^k p^k(\mathbf{x}, t); \)
\[
\nabla q_{ol}^{k+1}(\mathbf{x}, t) = \nabla q_{ol}^k(\mathbf{x}, t) + \varepsilon^k \nabla p^k(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma_{h0} \times [0, t_{max}].
\]

Step V: Set \( k = k + 1 \) and return to Step II.

### NUMERICAL DESIGN EXAMPLE

The salient features and performance of the adjoint methodology presented in the previous section are illustrated here through a numerical design example. In particular, the adjoint-based inverse design method presented earlier is employed to design the transient mold walls’ thermal boundary conditions for the reference solidification system considered earlier such that a stable interface growth is achieved (in the sense that Eq. (11) is marginally satisfied) with a growth velocity...
equal to that obtained in a solidification problem controlled only by heat and solute diffusion. As mentioned earlier in that section, we facilitate the realization of the design objectives by applying a strong horizontal magnetic field of strength $0.05 \ T$ ($H_a = 36.74$) such that the melt flow in the solidification system is substantially (but not fully) damped. This design example represents a preliminary attempt to calculate process conditions to achieve “diffusion-based” conditions in the presence of convection in the melt because of nonlinear forcing terms (in the current case, coupled buoyancy, thermocapillary, and electromagnetic melt convection). Eliminating the detrimental effects of coupled convective flow and achieving morphologically stable growth are issues of paramount importance in the processing of advanced materials with desired solidification microstructures.

Referring to the reference binary eutectic solidification problem presented in the reference binary eutectic alloy solidification problem section, we now pose the following inverse design problem:

Find the thermal boundary conditions on the left wall $x = 0$ and the right wall $x = 1$ such that with coupled thermocapillary, buoyancy, and electromagnetic convection in the melt, a vertical desired interface growth is achieved that is enforced to be morphologically stable.

Here, desired growth refers to a growth velocity $v_f$ corresponding to a solidification problem driven only by heat and solute diffusion, and the interface thermal gradient $G$ is chosen such that the stability condition given by Eq. (11) is marginally satisfied. Because the interfacial thermal gradient $G$ and growth velocity $v_f$ are the main macroscopic parameters controlling the form and scale of cast microstructures obtained in [36], we can also recast the inverse design objective in terms of achieving a desired solidification microstructure in the final product.

As has been outlined earlier, the inverse design eutectic solidification problem can be decomposed into two design subproblems—an IHCP in the solid domain and a inverse convection problem in the melt. In this article, we provide no further discussion on the IHCP defined in the solid region as this issue has been amply treated in several earlier references.

The inverse problem in the liquid domain solves for $q_{ol}(y, t)$ at $x = 1$ using the given freezing interface velocity $v_f(t)$ and the interface thermal gradient $G$. The desired freezing interface velocity $v_f(t)$ (see Figure 6a) is obtained by solving a direct solidification problem without the effects of melt convection, and the desired interface thermal gradient $G$ (see Figure 6b) is chosen using this interface velocity field such that the condition given in Eq. (11) is marginally satisfied. It is important to mention here that, because of the rapid transient associated with the solidification process at early times, a smooth transition (over the duration $\tau < 0.02$) to the desired heat flux $G$ was employed in the implementation to avoid numerical difficulties. An initial guess heat flux $q_{ol}^0(y, t) \equiv 0$ corresponding to the reference eutectic solidification problem was chosen to start the CGM algorithm. As in the reference solidification problem, we terminate the calculations at $t_{max} = 1.5$, at which time convection in the melt has practically died out and about 65% of the domain has solidified. Because the effects of convection are diminished, the end-condition problem associated with the adjoint method [8, 32] is practically unimportant.
(Recall that the adjoint method imposes an artificial condition for the adjoint temperature field at the final time, which in turn implies that, for each CGM iteration, the flux solution maintains its value from the initial guess solution.)

Within each CGM iteration, the direct, adjoint, and sensitivity problems are solved using the same finite element algorithms and solution methodologies as in the direct solidification problem. To avoid issues related to inconsistent derivatives, we also use the same spatial/temporal discretizations for the direct, adjoint, and sensitivity problems. The computational cost of solving the three subproblems at each CGM iteration (including the overhead associated with storing/retrieving the direct solution fields) is about 7 hours of CPU time on the AC3 velocity cluster provided by CTC. To damp out oscillations in the inverse solution because of error in the data, the $H^1$ regularized adjoint formulation introduced earlier is used with a regularization parameter $\gamma = 5 \times 10^{-4}$. Such a practice of applying some form of smoothing technique (either within the inverse algorithm or as a postprocessing operation) to obtain flux solutions that are optimal, while at the same time sufficiently smooth, is typical in inverse solidification/crystal growth simulations (see, for example, [37]).

The convergence of the CGM method is shown in Figure 7. The cost functional decreases very rapidly in the initial few iterations and then gradually reaches an asymptotic value. The norm of the gradient is also shown in the same plot. As is the case with the solution of other similar inverse problems [8, 32], the norm of the gradient does decrease with iterations, but not monotonically. The CGM iterations are terminated after the norm of the gradient $||J'(q^h)||$ is below the set tolerance of $10^{-3}$. Notice that the cost functional reaches an asymptotic value at a relatively high value of around 0.01, unlike our previous studies [10,11]. The main reason for this trend is the presence of a singular corner region in the flow that is unaffected by the control heat flux. It is expected that the use of a relatively finer mesh, which can resolve the corner flow more precisely, can help alleviate this problem.

Figure 6. The desired interface velocity $v_f(t)$ and the heat flux $G$ calculated through the solution of a "diffusion-based" problem.
The development of the heat flux profiles during the intermediate stages of the CG process are shown in Figures 8a–d. The optimal liquid-side flux $q_{ol}(y, t)$ obtained at the termination of the CG iterations is shown in Figure 8e. Note that the optimal heat flux profiles show the most heating very early. This strong heating flux has to be applied early in order to counteract the effects of coupled thermocapillary and buoyancy-driven fluid flow at very early stages of the solidification process in ensuring morphological stability.

Figure 8f shows the optimal solution $\bar{q}_{os}(y, t)$ of the IHCP in the solid region. It is obtained by the adjoint method using the solid-side interface heat flux (calculated using the Stefan condition and the prescribed growth velocity $v_f(t)$ and liquid-side interface flux $G$) and the equilibrium condition on the interface. It is the combined application of the heat fluxes $\bar{q}_{os}(y, t)$ and $\bar{q}_{ol}(y, t)$, that leads to the desired stable growth conditions.

**VALIDATION OF THE INVERSE DESIGN SOLUTION**

In this section, we evaluate the inverse design solution to check how close the desired design objectives have been met. To this end, we consider a direct eutectic solidification problem (including the simultaneous analysis of the solid and liquid phases) with the calculated optimal solid-side flux $q_{os}(y, t)$ applied on the left boundary $x = 0$ and the liquid-side flux $q_{ol}(y, t)$ applied on the right boundary $x = 1$. The
top and bottom walls are, as before, insulated. We refer to this problem as the optimal design eutectic-solidification problem. Here we compare the solution to this problem with that of the reference design problem and check if the objectives of stable desired growth are actually achieved under the conditions that thermodynamic equilibrium is satisfied on the solidifying interface.

To quantify the deviation of the calculated interface growth velocity $v_f(y, t)$ for the reference and optimal design solidification problems from the target (or desired) growth velocity, we define the standard deviation $\sigma_v(t)$ as follows:

$$\sigma_v(t) \equiv \left\{ \frac{1}{N} \sum_{i=1}^{N} \left[ |v_f(i, t)| - v_d(t) \right]^2 \right\}^{1/2}$$

(29)
Here, $|v_f(i, t)|$ is the magnitude of the interface velocity at the $i$th node and $v_d(t)$ is the desired growth velocity shown in Figure 6a. This quantity provides a measure of the deviation of the solid–liquid interface growth from the desired vertical interface growth. Notice the prominent decrease in the standard deviation $\sigma_v(t)$ in the case of the optimal design solution relative to the reference design problem (see Figure 9a). Figure 9b further illustrates this aspect by comparing the transient solid domain grids at early stages of the solidification process for the reference and optimal design solidification problems. It clearly demonstrates the positive effects of a strong magnetic field and optimally designed thermal boundary fluxes in achieving the desired vertical interface growth. Representative transient temperature, concentration, and flow fields (contours of isotherms, isoleths, and stream functions) corresponding to the optimal design eutectic solidification problem are illustrated in Figure 10. Because of the application of a strong heating flux on the right boundary $x = 1$, a temperature gradient is maintained even at times $t \approx t_{\text{max}}$. This thermal gradient is necessary to overcome the solutal undercooling to maintain a stable interface growth throughout the solidification process. A comparison of the temperature plots for the reference and optimal design solidification problems also provides an explanation for the higher values of $\sigma_v(t)$ observed in Figure 9a for the optimal design problem relative to the reference problem at times $t \approx t_{\text{max}}$. The reason for such a trend lies in the fact that, for the reference solidification system, all the superheat in the melt is lost by $t \approx t_{\text{max}}$, leading to an interface velocity that closely matches the desired “diffusion-based” growth velocity, but this is not the case in the optimal design problem. From the calculated results, although it appears that the interface growth velocity $v_f(t)$ for the reference solidification system deviates little from the desired growth velocity at times $t \approx t_{\text{max}}$, it is important to note that this deviation is only a numerical artifact and is not representative of the actual physical system because of the fact that the reference design solidification system turns unstable by about $t \approx 0.2$ (see Figure 4b). As is discussed below, however, this is not the case with the optimal design solution.

We next test the accuracy of the optimal design solution by checking if the condition given in Eq. (11) is satisfied. Figure 11a shows the dimensionless contours of $\Delta(y, t) \equiv G/|v_f| + m(C_E - C_o)/D_L$ as a function of the $y$-coordinate and time. As mentioned earlier $\Delta(y, t) \geq 0$ implies stable growth. As is clear from the plot, stable growth is achieved for the entire duration of solidification, confirming the realization of the design objectives. However, because the cost functional reaches an asymptotic value at a high value of around 0.01, the calculated contours of $\Delta(y, t)$ are significantly higher than the expected value of zero (recall that, because we impose $G$ to be such that $G/|v_f|$ marginally satisfies the condition given in Eq. (11), one would ideally expect $\Delta(y, t) \approx 0$ under the circumstance that the cost functional is sufficiently close to zero).

Finally, in Figure 11b we show the solid composition corresponding to the optimal design solution. Note the vertical uniformity in the solid composition in comparison to the stratification observed in the reference eutectic solidification problem shown in Figure 4a.
Figure 9. (a) Standard deviation $\sigma_v(t)$ for the optimal and reference design problems; (b) comparison of the solid domain grids at intermediate times $\tau = 0.1$ and $\tau = 0.4$ demonstrating the prominent reduction in interface curvature because of the application of the optimally calculated heat fluxes.
In this paper, a systematic adjoint formulation is presented for the design of two-dimensional directional binary eutectic solidification processes with melt flow driven by the combined effects of thermocapillary, buoyancy, and electromagnetic convection. The objective was to control the boundary thermal fluxes such that solidification proceeds with a desired flat interface morphology and under morphologically stable growth conditions. Stability in this work implies satisfaction

SUMMARY AND CONCLUSIONS

Figure 10. (a)–(c) Contours of the fluid stream function; (d)–(f) isotherms; and (g)–(i) composition for the optimal design solidification simulation. Simulation results are shown at dimensionless times $\tau = 0.1$, $\tau = 0.8$, and $\tau = 1.5$. 
Figure 11. (a) Examination of the constitutional stability assumption at the solid–liquid interface for the optimal design solidification problem. Dimensionless contours of $\Delta \equiv \frac{G}{|y|} + \frac{m(C_L - C_o)}{D_L}$ are displayed. Notice that stable growth is achieved for the entire duration of solidification; Contours plot of the solid composition (in wt% Germanium) for the optimal solidification design problem. Note the vertical uniformity in the solid distribution patterns obtained for the reference eutectic solidification problem.
of an a priori determined constraint on the ratio $G/|\psi_f|$. To ensure stable numerical results, an $H^1$-type regularization was incorporated in the adjoint-based design methodology. The implementation of the optimization problem of the inverse method is carried out using the CGM, whereas FEM techniques are used to solve the direct, adjoint, and sensitivity subproblems. The methodology was demonstrated using an example problem, and the numerical results were validated through the solution of a direct solidification problem with the application of the optimally designed fluxes.

The current study and some of our earlier work clearly demonstrate the need for improvement in the various computational methods used to solve the inverse fluid flow problem. Furthermore, these studies also emphasize the need for employing finer spatial discretizations in the direct simulations such that better accuracy and numerical resolution is achieved. To achieve these goals, we are considering the use of multiblock, multigrid methods to improve the performance of the various algorithms. Focused research efforts are also being directed toward extending the various computational methods to design solidification processes with continuum mushy zone solidification models. This would help in developing computational methods for the design of solidification/crystal growth processes with complicated geometries, and so on. With such a generic continuum direct model, other important design objectives, such as controlling the residual segregation in the solid, also can be considered. Efforts also are being directed towards including other design parameters such as the magnitude and orientation of the applied magnetic field into the inverse formulation. Several mathematical, modeling, and computational issues need to be addressed to achieve these important goals.

REFERENCES


