INVERSEFINITE ELEMENT TECHNIQUES FOR THE
ANALYSIS OF SOLIDIFICATION PROCESSES

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SUMMARY

This paper provides a finite element methodology (FEM) for the solution of several one-dimensional inverse solidification problems. In particular two design related problems will be addressed. The first one uses an inverse technique to calculate the boundary heat flux history that will achieve a specified velocity and flux at the freezing front. This front velocity and flux history can be appropriately selected so that the cast structure is controlled. The second problem is the calculation of the boundary heat flux and freezing front position, given appropriate estimates of the temperature field in a specified number of sensor locations (thermocouples) inside a solidifying body. Front fixing and front tracking FEM techniques are used for the solution of the first problem, while a fixed domain finite element formulation (enthalpy method) is used for the solution of the second one. The 'future information technique' is employed in both problems. A detailed analysis of the effect on the solution of the error in the data, amount of future information used, time step, number of sensors and their location and of other parameters in the solution will be examined via several numerical tests. Finally, further applications of such inverse methodologies on the control of casting processes will be mentioned.

INTRODUCTION

Inverse heat transfer problems have been the subject of intense research. Most of this effort has been concentrated in one-dimensional inverse heat conduction problems without phase changes. The inverse heat conduction problem usually refers to the problem of calculating the boundary heat flux and temperature in a solid given approximate measurements of the temperature at a specified number of sensor locations inside the solid. A rather extensive literature review can be found in Beck et al.

Inverse heat conduction problems with phase changes are the subject of this paper. An example is an inverse Stefan problem, where the interface velocity and location as well as the temperature field in the solid phase are to be predicted from the temperature history at specified sensor locations inside the solid phase. This problem, which has been previously analysed by Zabarás and Ruan and Katz and Rubinsky, has many applications in the design of welding processes. Further work on the subject of inverse heat transfer problems with a phase change includes that of Hsu et al., Frederic and Greif and Zabarás et al. This last reference presents a boundary element algorithm for the calculation of the boundary heat fluxes, given the heat fluxes on the freezing front as well as the freezing front velocity and location. Solution of this problem can be useful in controlling the cast structure by determining the boundary heat flux required to achieve certain values of front fluxes and velocity. This problem will be further analysed in this paper.

Most of the algorithms used to account for the ill-posed nature of these inverse problems include least squares techniques, regularization, filtering, dynamic programming and other
optimization methods. These methods have been used in conjunction with direct methodologies including finite difference, finite element and boundary element techniques. It should be emphasized that the numerical methods used to solve the direct problem, as is possibly required by the inverse methodology, do not play any important role in the accuracy of the inverse solution but they can be selected appropriately to simplify the involved computations.

In this paper, the 'future information' method introduced by Beck and co-workers\textsuperscript{1,7–10} will be used to analyse two distinct inverse solidification problems. The first one is similar to that presented in Zabaras et al.\textsuperscript{6} Two different techniques are used for its analysis, a front fixing one which immobilizes the freezing front with a proper space co-ordinate transformation and a front tracking one which continuously updates the mesh to account for the freezing front motion.

In the second problem of interest, the enthalpy method\textsuperscript{11} will be employed to calculate the boundary flux given temperature measurements at points inside a solidifying domain. The finite element method is employed in both problems. Several numerical tests are performed to investigate the effect on the solution of several parameters. The paper will conclude with a discussion on future directions and potential applications of inverse techniques to the design of casting processes.

**DEFINITION OF TWO INVERSE SOLIDIFICATION PROBLEMS**

Consider solidification in a region of length \( d \) occupied initially by liquid of temperature \( T_{l}(x) \), with \( T_{m} \) denoting the melting temperature (Figure 1). Let \( h(t) \) be the position of the freezing front at time \( t \), where \( h(0) = 0 \) and \( T(x, t) \) is the temperature at time \( t \) and position \( x \). The conductivity \( K \), density \( \rho \) and specific heat \( c \) are considered to be temperature independent. The subscripts \( S \) and \( L \) are introduced to denote solid and liquid phases, respectively, while the subscripts \( o \) and \( m \) denote a fixed or a moving (freezing front) boundary.

\[
q_{ol} = -K_{l} \frac{\partial T_{l}}{\partial x}(d, t)
\]

\[
q_{lm} = +K_{l} \frac{\partial T_{l}}{\partial x}(h(t), t)
\]

\[
q_{ms} = -K_{s} \frac{\partial T_{s}}{\partial x}(h(t), t)
\]

\[
q_{os} = +K_{s} \frac{\partial T_{s}}{\partial x}(0, t)
\]

Figure 1. Geometry of uniaxial solidification
The governing equations of heat conduction in the above solidifying body can be written as follows:

\[
K_S \frac{\partial^2 T_S(x, t)}{\partial x^2} = \rho \frac{\partial T_S(x, t)}{\partial t} \quad 0 \leq x \leq h(t) \tag{1}
\]

\[
K_L \frac{\partial^2 T_L(x, t)}{\partial x^2} = \rho \frac{\partial T_L(x, t)}{\partial t} \quad h(t) \leq x \leq d \tag{2}
\]

\[
K_S \frac{\partial T_S(h(t), t)}{\partial x} - K_L \frac{\partial T_L(h(t), t)}{\partial x} = \rho \mathcal{L} \dot{h}(t) \tag{3}
\]

\[
T_S(h(t), t) = T_L(h(t), t) = T_m \tag{4}
\]

\[
h(0) = 0 \tag{5}
\]

\[
T(x, 0) = T_m(x) \tag{6}
\]

where \( \mathcal{L} \) is the latent heat of fusion, \( \dot{h}(t) \) the freezing front velocity at time \( t \) and equation (3) expresses a heat energy balance at the freezing front.

A direct problem can now be defined as follows: Given the melting temperature \( T_m \), the initial conditions (equations (5) and (6)), and proper boundary temperature or flux conditions at \( x = 0 \) and \( x = d \) (see Figure 1), calculate the temperature field \( T(x, t) \) for all \( x \) \((0 \leq x \leq d)\) and \( t \), as well as the freezing front velocity and location history.

Many methods of solution have been proposed for the solution of the above problem. Crank identifies these methods as fixed domain, front fixing, front tracking and analytical. In the fixed domain methods, for example the enthalpy method, appropriate heat source terms are introduced to account for equation (3) and a single differential equation is solved over the whole domain (solid and liquid). In the front fixing methods the front is fixed with a proper co-ordinate transformation. For example with \( \zeta = x/h(t) \) the front is always stationary at \( \zeta = 1 \). Such transform methods introduce complications since the front position is not specified from the outset, but rather is part of the solution of the problem. However, for design problems where the front position is specified \( a \ priori \), it will be shown that transform techniques offer significant advantages. Front tracking techniques involve deforming and/or moving finite elements or finite difference grids. The mesh is continuously moving to adapt to the freezing front motion. Finally there is only a limited number of one-dimensional and two-dimensional wedge space analytical solutions. In this paper two distinct inverse solidification problems are of interest. These problems are defined as follows.

**Inverse problem A**

Given the melting temperature \( T_m \), the front velocity \( \dot{h}(t) \) and flux \( q_{ns}(t) = -K_S \frac{\partial T_S(h(t), t)}{\partial x} \), solve equations (1)–(6) for the temperature field \( T(x, t) \). Note that the specified values of the front velocity \( \dot{h}(t) \) and flux \( q_{ns}(t) \), can be used in equation (3) to specify the flux \( q_{ml}(t) = K_L \frac{\partial T_L(h(t), t)}{\partial x} \) in the liquid side of the freezing front.

**Inverse problem B**

Given the melting temperature \( T_m \) and thermocouple measurements of the temperature field at \((N + 1)\) locations, as \( T(x_k, t) = Y_k(t), k = 1, 2, \ldots, N + 1 \), solve equations (1)–(6) for the temperature field \( T(x, t) \), where for simplicity is assumed that \( x_{N+1} = d \).
For both the above problems the material properties are assumed known. The boundary fluxes \( q_{os}(t) = K_S \frac{\partial T_S(0, t)}{\partial x} \) and \( q_{ntl}(t) = -K_L \frac{\partial T_L(d, t)}{\partial x} \) (see Figure 1), are considered as primary variables. Obviously once the boundary fluxes are known, the calculation of the temperature field \( T(x, t) \) is equivalent to solving a direct problem. The above defined problems are ill-posed, since small changes in the given data can result in a significant change in their classical solution. Inverse problem A can have many potential applications in the design of casting processes. Specifically, the freezing front velocity and fluxes can be selected in such a way that a desired cast structure is achieved.\(^{14}\) Further, solution of problem A can be used to control the freezing front motion, optimize the time of casting and prevent choking of the liquid flow.\(^6\) Inverse problem B is similar in nature to the inverse heat conduction problems addressed by Beck et al.,\(^1\) but it is a more difficult one since it involves a phase change material and a moving boundary.

**SURFACE HEAT FLUX DETERMINATION FROM GIVEN FLUX AND VELOCITY AT THE FREEZING FRONT (INVERSE PROBLEM A)**

(i) A front fixing finite element analysis

For demonstration of ideas, let us concentrate on the solid phase, where the heat conduction is governed by equation (1) in the moving region \( 0 \leq x \leq h(t) \). To fix the location of the freezing front one can introduce the spatial transformation \( \zeta = x/h(t) \). Such a transformation can be particularly attractive in cases where the front velocity is a priori known, like in the inverse problem A under consideration. The transformed problem in the solid phase is then governed by the following equations:

\[
K_S \frac{\partial^2 T_S(\zeta, t)}{\partial \zeta^2} - \rho c_s h^2 \left( \frac{\partial T_S(\zeta, t)}{\partial t} - \frac{\zeta}{h} \frac{\partial T_S(\zeta, t)}{\partial \zeta} \right) = 0 \quad 0 \leq \zeta \leq 1 \quad (7)
\]

\[
T_S(\zeta, t) = T_m \quad \zeta = 1 \quad (8)
\]

\[
- K_S \frac{\partial T_S(\zeta, t)}{\partial \zeta} = h(t) q_{ns}(t) \quad \zeta = 1 \quad (9)
\]

\[
K_S \frac{\partial T_S(\zeta, t)}{\partial \zeta} = h(t) q_{os}(t) \quad \zeta = 0 \quad (10)
\]

Dividing the region \( 0 \leq \zeta \leq 1 \) into \( E \) finite elements and \( M \) nodes and applying a Galerkin weak formulation to equation (7) leads to the following assembled system of equations:\(^{15,16}\)

\[
C_{ij} \frac{\partial T_i}{\partial t} + K_{ij} T_j = F_i \quad i, j = 1, 2, \ldots, M \quad \text{(sum on j)} \quad (11)
\]

where

\[
C_{ij} = \sum_e C_{ij}^e = \sum_e \int_{\Omega_e} \rho c_s h^2(t) \Phi_i^e(\zeta) \Phi_j^e(\zeta) \, d\zeta \quad (12)
\]

\[
K_{ij} = \sum_e K_{ij}^e = \sum_e \int_{\Gamma_e} K_S \frac{\partial \Phi_i^e(\zeta)}{\partial \zeta} \frac{\partial \Phi_j^e(\zeta)}{\partial \zeta} \, d\zeta \quad (13)
\]

\[
- \sum_e \int_{\Omega_e} \rho c_s h(t) \dot{h}(t) \Phi_i^e(\zeta) \frac{\partial \Phi_j^e(\zeta)}{\partial \zeta} \, d\zeta
\]
\[ F_i = \sum_e F_i^e = -\sum_e h(t) q_{est}(t) \Phi_i^e(0) - \sum_e h(t) q_{act}(t) \Phi_i^e(h(t)) \]  \hspace{1cm} (14) 

and \( C_{ij} \) and \( K_{ij} \) are referring to the element \( e \), occupying the space \( \Omega_e(t) \), with \( \Phi_i^e \) and \( \partial \Phi_i^e(\xi) / \partial \xi \) the one-dimensional space shape functions and their derivatives, respectively.

The following time integration scheme is introduced\(^1\) for equation (11):

\[
\frac{[C]}{\Delta t} + \beta [K]\{T\}_{t+\Delta t} = \frac{[C]}{\Delta t} - (1 - \beta)[K]\{T\}_t + (1 - \beta)\{F\}_t + \beta\{F\}_{t+\Delta t} \hspace{1cm} (15)
\]

where \( 0.5 \leq \beta \leq 1 \) and the matrices \([C]\) and \([K]\) above are calculated using the velocity \( h(t) \), at time \( t = (1 - \beta)t + \beta(t + \Delta t) \). In a direct Stefan problem, the front velocity is unknown and equation (15) must be solved iteratively in time together with proper boundary conditions.

An equation similar to equation (15) can be derived for the liquid phase. The analysis follows the same steps as in the solid phase and it will not be repeated here.

(ii) A front tracking finite element analysis

To demonstrate the method, let us again concentrate on the solid phase. The moving region \( 0 \leq x \leq h(t) \) is divided into a fixed number of finite elements with nodes moving with time and following the motion of the interface. This assumption\(^2, 18-22\) makes the shape functions to implicitly depend on time through the nodal co-ordinates. For example, for each finite element \( e \), one can write the following equation:

\[ T(x, t) = T_i^e(t) \Phi_i^e(x, t) \hspace{1cm} \text{(sum on } i) \]  \hspace{1cm} (16)

where \( T_i^e(t) \) are the nodal temperatures, \( \Phi_i^e(x, t) \) the element shape functions and \( x \) is a spatial point lying inside the element. In equation (16), summation on \( i \) is implied \( (i = 1, 2, \ldots, M^e) \), where \( M^e \) is the number of nodes in the element \( e \). By assuming an isoparametric transformation of the space \( x \) to the time independent space \( \xi \), with \( -1 \leq \xi \leq 1 \), one can write

\[ x = X_i(t) \Phi_i(\xi) \hspace{1cm} \text{(sum on } i, i = 1, M^e) \]  \hspace{1cm} (17)

Let us now assume that the space occupied by the solid phase is divided into \( E \) elements with \( M \) nodes. Then, at each time \( t \), one can employ a weak Galerkin formulation for equation (1) and using equations (16) and (17), write the following discretized equations:\(^9\)

\[
C_{ij} \frac{\partial T_i}{\partial t} + (B_{ij} + K_{ij})T_j = F_i \hspace{1cm} i = 1, M, \hspace{.5cm} j = 1, M \hspace{1cm} \text{(sum on } j) \]  \hspace{1cm} (18)

where

\[
B_{ij} = \sum_e B_{ij}^e = -\sum_e \int_{\Omega_e} \rho c \frac{dx}{dt} (x, t) \Phi_i^e(x, t) \frac{\partial \Phi_j^e(x, t)}{\partial x} \frac{dx}{dt} \hspace{1cm} (19)
\]

while the expressions for \([K], [C] \) and \([F]\) are of the same form as for non-moving finite elements and are given in several finite element texts.\(^5, 6\) Note that the integrations involved in equation (19) (and in the calculation of the other matrices and vectors in equation (18)) are performed over the time dependent length \( \Omega_e(t) \) of each element \( e \). Obviously, \( \sum \Omega_e(t) = h(t) \), i.e. the space occupied at time \( t \) by the solid phase. The matrix \([B]\) accounts for the motion of the nodes. It is important to note here that the finite element nodes are moving only artificially (no actual material motion exists). Therefore, it left to us to decide the optimum way the nodes should move. In this work, the nodes are moving such that a uniform mesh is always present at \( 0 \leq x \leq h(t) \).
A time marching scheme similar to that of equation (15) can be proposed for equation (18) where \([K] + [B]\) is used instead of \([K]\). As with the front fixing method, all the involved matrices are functions of the interface velocity and position, which for the inverse problem of interest are known a priori. In the numerical implementation of this technique, the front position was used as a main variable, while the interface velocity was calculated from the front position as \(h(t) = (h(t + \Delta t) - h(t))/\Delta t\).

(iii) Inverse algorithm

Again, for demonstration of ideas, the inverse problem in the solid phase is undertaken. The freezing interface temperature \(T_m\), velocity \(h(t)\) and flux \(q_{os}\), are assumed known while the main unknown is the boundary flux \(q_{os}\). Let us consider a time stepping process, \(t_F, t_F, \ldots\), and let us denote the boundary flux as \(q_{os}^{F+i-1} = q_{os}(t_F+i-1)\), the finite element nodal temperatures as \(T^{F+i-1} = \{T(t_F+i-1)\}\) and the calculated temperature at the Mth node \((x = h(t))\) as \(T^{F+i-1}_M = T_M(t_F+i-1)\).

The boundary fluxes \(q_{os}\) as well as the nodal temperatures \(T^J\), \(J < F\), are assumed known.

To calculate \(q_{os}\), it is temporarily assumed that

\[
q_{os}^F = q_{os}^{F+1} = \ldots = q_{os}^{F+r-1}
\]

for \((r - 1)\) future steps. This assumption, attributed to Beck,\(^1\) will add stability to this ill-posed problem and it will make a sequential calculation of \(q_{os}\) possible.

Let \(q_{os}^r\) be an iterative approximation of \(q_{os}^F\) (for example at the beginning of iterations \(q_{os}^{F-1}\)), then one can write

\[
T^{F+i-1}_M = T^{F+i-1}_M + \left[ \frac{\partial T^{F+i-1}_M}{\partial q_{os}^F} \right]_* (q_{os}^F - q_{os}^r)
\]

(21)

where the sensitivity coefficients, \(\left[ \frac{\partial T^{F+i-1}_M}{\partial q_{os}} \right]_*\), express the change of the temperature on the Mth finite element node with a unit change of the boundary flux \(q_{os}\). These coefficients are calculated using the fluxes \(q_{os}^F - q_{os}^{F+1} = \ldots = q_{os}^{F+r-1}\). The starred temperatures, \(T^{F+i-1}_M\), \(i = 1, r\), result by solving a direct problem on the time interval \(t_F \leq x \leq t_{F+r-1}\), with the flux \(q_{os}\) as the boundary condition at \(x = 0\) and equation (9) as the flux boundary condition on the freezing front \((x = h(t))\).

To calculate an updated value of the flux \(q_{os}\), the freezing interface is treated as the location of a perfect temperature sensor with \(T(h(t), t) = T_m\) for all time. Then, one can minimize with respect to the flux \(q_{os}\) the following error:

\[
\min_{q_{os}} E = \frac{1}{2} \min q_{os} \sum_{i=1}^{r} (T^{F+i-1}_M - T_m)^2
\]

(22)

where \(T^{F+i-1}_M\) is calculated using equation (21). Note that, even though the above error is defined over \((r - 1)\) steps, owing to the assumption (20) it is a function only of the flux \(q_{os}\). Using equation (21) and differentiating the above functional with respect to \(q_{os}\) leads to

\[
q_{os}^F = q_{os}^* + \frac{\sum_{i=1}^{r} \left[ \frac{\partial T^{F+i-1}_M}{\partial q_{os}} \right]_* (T_m - T^{F+i-1}_M)}{\sum_{i=1}^{r} \left[ \frac{\partial T^{F+i-1}_M}{\partial q_{os}} \right]_*^2}
\]

(23)
The above equation can be used to update the flux \( q_{os} \) assuming that the sensitivity coefficients and the starred temperatures can be calculated.

The following approximation is used for the sensitivity coefficients:

\[
\left[ \frac{\partial T_{M}^{F_{r+1}}}{\partial q_{os}^{F}} \right]_{r} = \frac{T_{M}^{F_{r+1}} - T_{M}^{F_{r}}} {q_{os}^{F} - q_{os}^{F} (1 + \varepsilon)}
\]  \( (24) \)

where \( \varepsilon \approx 10^{-3} \) and \( T_{M}^{F_{r+1}} \) is the temperature on the \( M \)th node calculated using the direct algorithm (for example equation (15)), with the flux \( q_{os}^{F} (1 + \varepsilon) \) as the boundary condition at \( x = 0 \) (constant on the time interval \( t_{F} \leq x \leq t_{F+r+1} \)) and the given flux \( q_{os}(t) \) at the freezing front.

**(iv) Summary of the algorithm**

In the inverse problem in the solid phase the following algorithm is used. For \( F = 1, 2, \ldots \cdot \)

1. Start iteration \( \text{iter} = 1, 2, \ldots, \text{imax} \)
2. Approximate \( q_{os}^{F} \) with the previous estimate (at first iteration use \( q_{os}^{F} = 1 \))
3. Assume \( q_{os}^{F} = q_{os}^{F+1} = \ldots = q_{os}^{F+r-1} \)
4. Solve equation (15) for \( T_{M}^{F_{r+1}} \), \( i = 1, 2, \ldots, r \) (Direct problem)
5. Calculate sensitivity coefficients (equation (24))
6. Update the flux \( q_{os}^{F} \) (equation (23))
7. If \( |(q_{os}^{F} - q_{os}^{F})/q_{os}^{F}| > \delta \), where \( \delta \) is a given tolerance, take \( q_{os}^{F} = q_{os}^{F} \) and continue iterations, otherwise go to the next time step.

Since as time passes the front (sensor) is moving away from the boundary \( x = 0 \) where the flux is needed, it is expected that the accuracy of the above (and practically any other) algorithm will deteriorate with time.

The inverse problem in the liquid phase, on the other hand, consists in solving for the flux \( q_{os} \) given the freezing interface temperature \( T_{m} \), velocity \( h(t) \) and flux \( q_{nl}(t) \) at \( x = h(t) \). The algorithm is the same as that in the solid phase, but in contrast to the inverse problem in the solid phase, it should be recognized that the inverse problem here is a rather difficult one. Indeed, at time zero the distance between the sensor (at \( x = 0 \)) and the calculation point (at \( x = d \)) is the maximum possible and it becomes obvious that, for large \( d \) and early time, the algorithm can fail to recognize the correct boundary conditions. This point will be further investigated through numerical examples.

**(e) Numerical examples**

To examine the effectiveness of the above mentioned algorithms in the solution of inverse solidification problems of type A, two examples will be considered. The first one concentrates on the solid phase and will be solved using the front fixing method.

Consider solidification in a semi-infinite region, initially occupied with liquid at \( T_{in}(x) = 0 \), with material properties \( K_{s} = 1, \rho = 1, c_{s} = 1, \mathscr{L} = 0.5 \) and \( T_{m} = 0 \) (dimensionless quantities are used in this section). The desired freezing front velocity is \( h_{\text{exact}}(t) = 2 \) (so \( h_{\text{exact}}(t) = 2t \)), while the interface fluxes are (see equation (3)) \( q_{os}(t) = -1 \) and \( q_{nl}(t) = 0 \). The analytical solution of this inverse problem was given by Stefan and it is reported by Carslaw and Jaeger\(^{11}\) as follows:

\[
q_{os}(t) = e^{4t}
\]  \( (25) \)

\[
T_{os}(t) = \frac{1}{2} (1 - e^{4t})
\]  \( (26) \)
The same inverse problem was examined recently by Zabaras et al. using the boundary element method. The problem here is simulated with a FEM implementation of the front fixing method presented earlier, using 10 linear elements. It is expected that very good accuracy should be achieved at early time where the distance between the sensor \( x = h(t) \) and the calculation point \( x = 0 \) is small, while as time passes the solution should become unstable and the algorithm should fail to recognize the correct boundary condition. Figure 2 presents the calculated flux at \( x = 0 \) using no future information and three different time steps. Indeed it can be clearly seen that the calculated boundary flux becomes unstable at early time in the case of small time steps rather than large ones (unstable regions are not shown in Figure 2). To further investigate the stability of the algorithm, an approximate interface velocity and location to the desired ones are assumed. Specifically it is assumed that \( \dot{h}(t) = h_{\text{exact}}(1 + \gamma w) \) and \( h(t) = h_{\text{exact}}(1 + \gamma w) \), where \( w \) is a random number on the interval \([-1, 1]\) and \( \gamma \) is the per cent of error desired. Figure 3 demonstrates the effect of the time step \( \Delta t \) in a case with 2 per cent error \( (\gamma = 0.02) \) and no future information \( (r = 1) \). It is clear that the solution becomes less accurate and less stable in comparison to the case reported in Figure 2. To demonstrate the effect of future information, Figures 4 and 5 show the

![Figure 2. Boundary heat flux \( q_{\text{in}} \) as a function of time for various time steps with exact data (front fixing method).](image_url)

![Figure 3. Boundary heat flux \( q_{\text{in}} \) as a function of time for various time steps with inexact data (front fixing method).](image_url)
boundary flux and temperature for the same case as before but with one future step ($r = 2$). It can be concluded that, in the case of approximate data, the stability and accuracy of the system are drastically improved when future information is used. However, note that when $r > 3$ was used, significant bias was introduced in the solution, since at future steps the front is further away from the fixed boundary and the future information does not contribute to the accuracy and stability of the calculated flux.

The front tracking method was also used to solve the above problem. The results were of very similar nature to those reported above.

The second example concentrates on the liquid phase. The results for this example will be given using the deforming finite element technique (front tracking method). Solidification is considered of a liquid initially supercooled at $T_{in} = -1$ ($T_m = 0$) in a region of length $d = 1$, with $K_L = 1$, $\rho = 1$, $c_L = 1$, $\mathcal{S} = 2$, front velocity $\hat{h}_{exact}(t) = 0.432756/\sqrt{t}$ and front location
\[ h_{\text{exact}}(t) = 0.865512 \sqrt{t} \]
The interface fluxes are given as \( q_{\text{mL}}(t) = 0 \) while \( q_{\text{ml}}(t) \) is calculated through equation (3). The solidifying part of the region remains at the melting temperature at all time. The analytical solution to this problem is given as \(^{13}\)

\[
q_{\text{at}}(t) = 1.0437602 \frac{1}{\sqrt{t}} e^{-1/4t}
\]

\[
T_{\text{at}}(t) = -1 + 1.850017 \text{erfc} \frac{1}{2\sqrt{t}}
\]

where \( \text{erfc} \) is the complementary error function.

The FEM mesh consists of 10 linear elements which deform with time in such a way that a uniform mesh is always preserved. \(^2\) Figure 6 shows the calculated boundary flux using the exact desired velocity and interface flux data, one future step and two different time steps, \( \Delta t = 0.1 \) and \( \Delta t = 0.2 \). Both solutions appear stable but the small time step solution is less accurate at early

![Figure 6. Boundary heat flux \( q_{\text{at}} \) as a function of time for various time steps (front tracking method)](image)

![Figure 7. Boundary heat flux \( q_{\text{at}} \) as a function of time for various future time steps (front tracking method)](image)
time when the distance of the freezing front from the calculation point \((x = d)\) is large. A qualitative comparison of Figures 2 and 6 shows the different nature of the inverse problem in the solid and liquid phases. The error for the early time solution in the solid phase is very small, while the error for the solution in the liquid phase appears to be as high as 30 per cent. Figure 7 shows that for a smaller time step, a higher value of \(r\) is required for accurate solution. It is clear that the important factor is the total time \((r\Delta t)\), which is therefore used in the minimization process (liquid version of equation (23)), rather than \(r\) itself. Finally, Figures 8 and 9 indicate that increasing \(r\) can be an efficient method for handling cases with error in the given data. The interface location was assumed to be \((1 + 0.04 w)\) times the desired location \((h_{\text{exact}})\) given earlier.

The interface velocity necessary for the calculations was determined numerically (using a finite difference approximation) from the approximately given interface position.

Finally, it should be mentioned that the results obtained using the front fixing method were similar to those shown above.

Figure 8. Boundary heat flux \(q_{\text{el}}\) as a function of time for various future time steps with inexact data (front tracking method)

Figure 9. Boundary temperature \(T_{\text{el}}\) as a function of time for various future time steps with inexact data (front tracking method)
By means of the ill-posed character of the above problems, a small enough time step will always lead to an unstable behaviour of the method, causing large errors in the calculated boundary flux. The enlargement of the number of future time steps was able to stabilize this phenomenon. Nevertheless, with a possible smaller time step and the same \( r \), the method will again exhibit an unstable behaviour. The correct numerical solution of these problems needs a balancing between the smallness of the time step and the number of future time steps. The numerical results presented in this section (Figures 2-9) show that stability cannot only be achieved by an increase of the number of future steps but also by an enlargement of the time step. In general, the amount of future information used depends on the amount of error in the given data. The parameter \( r \) should be kept small to avoid bias when data with small (or without) error are used.

**SURFACE HEAT FLUX DETERMINATION FROM GIVEN THERMOCOUPLE TEMPERATURE MEASUREMENTS (INVERSE PROBLEM B)**

(I) *An enthalpy formulation of the direct problem.*

The so-called fixed domain methods are commonly chosen techniques for the numerical solution of phase change problems. The freezing front flux condition (equation (3)) is incorporated into a new form of the governing equations, which is valid over the whole fixed domain (solid and liquid). The front location and velocity do not explicitly appear in the formulation, and they are calculated after solving the problem using post-processing operations. The enthalpy is the sum of sensible and latent heat contents and for Stefan problems (isothermal freezing front) can be defined as follows:

\[
H = \rho c_S (T - T_o) \quad (T < T_m) \tag{29}
\]

\[
H = \rho c_S (T_m - T_o) + \rho \mathcal{L} + \rho c_L (T - T_m) \quad (T \geq T_m) \tag{30}
\]

where \( T_o \) is a reference temperature.

Even though emphasis here is given to inverse Stefan problems, let us consider that freezing occurs over the finite temperature interval \([T_m - \Delta T, T_m + \Delta T]\). In this case the enthalpy function can be defined as

\[
H = \rho c_S (T - T_o) \quad (T \leq T_{m1}) \tag{31}
\]

\[
H = \rho c_S (T_{m1} - T_o) + \rho \mathcal{L} \frac{(T - T_{m1})}{2\Delta T} + \rho c_m (T - T_{m1}) \quad (T_{m1} \leq T \leq T_{m2}) \tag{32}
\]

\[
H = \rho c_S (T_{m1} - T_o) + \rho \mathcal{L} + \rho c_m (2\Delta T) + \rho c_L (T - T_{m2}) \quad (T \geq T_{m2}) \tag{33}
\]

where \( T_{m1} = T_m - \Delta T \) and \( T_{m2} = T_m + \Delta T \). \( c_m \) is the specific heat at the freezing range (here \( c_m = (c_S + c_L)/2 \)) and \( \Delta T \) is a temperature half range over which the phase change occurs. Note again that the interest of this work is in the case \( \Delta T = 0 \) and temperature independent thermal properties.

As will be shown, small \( \Delta T \) can add stability to the numerical system, while at the same time, since it is small, it will not significantly alter the Stefan problem. Stefan problems exhibit step changes in \( H \) which often cannot be handled easily in numerical implementations.

It can be shown\(^1\) that the governing equation for the Stefan problem can now take the form

\[
\frac{\partial}{\partial x} \left( K \frac{\partial T(x,t)}{\partial x} \right) = \epsilon_* \frac{\partial T(x,t)}{\partial t} \quad 0 < x < d \tag{34}
\]
where the effective heat capacity \( c_* \) is defined as

\[
c_* = \frac{dH}{dT}
\]

while the conductivity \( K \) is equal to \( K_s \) when \( T < T_{m1}, K_L \) when \( T > T_{m2} \) and \( (K_s + K_L)/2 \) for \( T_{m1} \leq T \leq T_{m2} \).

A direct calculation of the effective heat capacity is possible using equations (35) and (31)–(33). However, when this is used severe restrictions must be imposed on the discretization grid and time step.\(^{23}\)

In this paper the averaging technique proposed by Lemmon\(^ {11}\) will be followed. More specifically, the effective heat capacity \( c_* \) is evaluated as

\[
c_* = \frac{\partial H(x, t)}{\partial x} \frac{\partial x}{\partial T(x, t)}
\]

Considering a finite element discretization of the enthalpy and temperature field as follows,

\[
H(x, t) = H_i^e(t) \Phi_i(x) \quad \text{(sum on } i, i = 1, M^e)\]
\[
T(x, t) = T_i^e(t) \Phi_i(x) \quad \text{(sum on } i, i = 1, M^e)\]

where \( T_i^e(t) \) and \( H_i^e(t) \) are the nodal values of the temperature and enthalpy field, respectively, it becomes clear that equation (36) gives an effective heat capacity which is representative for the whole finite element.

A Galerkin formulation for this modified problem takes a discretized form similar to that given by equation (11), with the 'mass' matrix \( [C] \) calculated using equations (36)–(38) and where for the calculation of the stiffness matrix \( [K] \) the thermal conductivity is defined as was explained before.

In a direct algorithm given the boundary fluxes or temperatures at \( x = 0 \) and \( x = d \), one can employ an iterative scheme and march forward in time in order to calculate the nodal temperature history. With known nodal temperatures one can interpolate the temperature field to calculate the location \( x \) where the temperature \( T(x, t) = T_m \) (freezing front location).

(ii) Inverse algorithm

The main goal here is the calculation of the boundary flux \( q_{ds} \), the temperature field \( \{T\} \) and the history of the interface motion given the temperature field in \( N \) sensor locations \( x_k, k = 1, 2, \ldots, (N + 1) \) with \( x_N + 1 = d \). For clarity of the presentations it is assumed that \( x_1 < x_2 < \ldots < x_N + 1 \). The finite element nodes are arranged in such a way that there is always a node lying on each sensor location. For time greater than the arrival time of the freezing front at the first sensor, one can separate the problem into a direct phase change problem in the region \( x_1 \leq x \leq d \) and in an inverse (fixed phase) problem in the solid region \( 0 \leq x \leq x_1 \). Nevertheless, in this work the problem will be treated as an inverse problem in the whole region until complete solidification occurs.

The algorithm here proceeds similarly to the inverse algorithms reported earlier. However, the sensor measurement \( Y_{N+1} \) is treated as a temperature boundary condition at \( x = d \) and the error
to be minimized is modified as follows:

$$\min \sum_{q_{os}} \sum_{i=1}^{r} w_i \sum_{k=1}^{N} (Y_k^{F+i-1} - T_k^{F+i-1})^2$$

(39)

where $w_i$, $i = 1, 2, \ldots, r$ represent optimization weights corresponding to each future time step $i$ (here $w_i = 1$), $k$ refers to each sensor location and the rest of the notation is as before.

In this work, for each $i$, $i = 1, 2, \ldots, r$, we assume the following:

$$q_{os}^{F+i-1} = \frac{q_{os}^F}{b_i}$$

(40)

where

$$b_i = \sqrt{1 + (i - 1) \frac{\Delta t}{t_f}}$$

(41)

This behaviour is very common for many phase change problems and a similar idea has been used previously for the solution of some other inverse Stefan problems.\textsuperscript{2} It correctly predicts rapidly changing $q_{os}$ flux at small $t$, when freezing suddenly starts at $x = 0$, while it takes an asymptotic form at later time. This assumption (equations (40–41)) is valid for both $q_{os}^{F+i-1}$ and $q_{os}^{F+i-1}$, $i = 1, 2, \ldots, r$, and is different from the one used for the solution of inverse problem A where it was assumed that $b_i = 1$.

As in inverse problem A, at each sensor location one can write that

$$T_k^{F+i-1} = T_k^{F+i-1} + X_{k}^{F+i-1} (q_{os}^F - q_{os}^{F+i})$$

(42)

where the sensitivity coefficients $X_{k}^{F+i-1}$, $k = 1, 2, \ldots, N$ and $i = 1, 2, \ldots, r$ are defined as

$$X_{k}^{F+i-1} = \left[ \frac{\partial T_k^{F+i-1}}{\partial q_{os}^F} \right]_n$$

(43)

These sensitivity coefficients express the change of temperature at each sensor location for a unit change of the boundary heat flux $q_{os}^F$. The calculation of such sensitivity coefficients follows steps similar to those reported in the previous inverse problem A. Performing the minimization in equation (39), one can write

$$q_{os}^F = q_{os}^F + \sum_{i=1}^{r} w_i \sum_{k=1}^{N} X_{k}^{F+i-1} (Y_k^{F+i-1} - T_k^{F+i-1})$$

$$+ \sum_{i=1}^{r} w_i \sum_{k=1}^{N} (X_{k}^{F+i-1})^2$$

(44)

with $q_{os}^F$ an approximation to the boundary heat flux $q_{os}$ at time $t = t_f$.

The numerical algorithm is in principle the same as that reported for inverse problem A and it will not be repeated here.

**(iii) Numerical results**

Consider solidification in a semi-infinite region initially occupied with liquid at $T(x, 0) = 4°C$. The material properties are given as $\rho_{cs} = 0.49$ cal/°C cm$^3$, $K_s = 9.6 \times 10^{-3}$ cal/cm sec°C, $\rho_{cl} = 0.62$ cal/°C cm$^3$, $K_l = 6.9 \times 10^{-3}$ cal/cm sec°C, $\rho \mathcal{L} = 19.2$ cal/cm$^3$ and $T_m = 0°C$.\textsuperscript{19} The boundary $x = 0$ is cooled with $T(0, t) = -10°C$.\textsuperscript{19}
The analytical solution of this problem is given as

\[ T_{\text{exact}}(x, t) = \frac{T_m - T(0, t)}{\text{erf}(g)} \text{erf} \left( \frac{x}{2 \sqrt{\frac{\rho c_s}{K_{sf}}} \sqrt{g t}} \right) + T(0, t) \quad \text{for } x \leq h(t) \quad (45a) \]

\[ T_{\text{exact}}(x, t) = T(x, 0) - \frac{T_m}{\text{erfc} \left( \frac{x}{2 \sqrt{\frac{\rho c_s}{K_{sf}}} \sqrt{g t}} \right)} \quad \text{for } x > h(t) \quad (45b) \]

\[ h(t) = 2g \sqrt{\frac{K_{sf}}{\rho c_s}} \quad (45c) \]

and

\[ q_{\text{es}}(t) = \frac{T_m - T(0, t)}{\text{erf}(g)} \sqrt{\frac{K_{sf} c_s}{\pi t}} \quad (46) \]

where \text{erfc} is the complementary error function and \( g = 0.30730548 \).\textsuperscript{13}

Let us now reverse this direct problem and consider a finite region \((0, d)\) with \(d = 1\) cm, where two thermocouples are embedded at \(x = x_1 = 0.3\) cm and \(x = d\).

The measurement at \(x = d\) is assumed to be the exact one given by equations (45), i.e. \(Y_2(t) = T_{\text{exact}}(d, t)\), while for the first sensor an additive error is considered:

\[ Y_1(t) = T_{\text{exact}}(d, t) + w \quad (47) \]

where again \(w\) is a random number on the interval \([-1, 1]\).

Five quadratic finite elements were used for the analysis and the freezing half interval was taken as \(\Delta T = 0.15^\circ\text{C}\). In the following graphs the temperature is in °C, the boundary heat flux in cal/cm² sec, the front location in cm and the time in seconds.

Figures 10 and 11 show the boundary flux and the interface position history for cases with two different time steps and the same amount of future information \(r = 4\). Both cases appear stable, but the case with \(\Delta t = 2\) sec gives more accurate boundary flux. Also it becomes clear that the solution error is significant up to time slightly larger than the arrival time of the freezing front at the sensor location. Figures 12–14 demonstrate the effect of the sensor location \(x_1\), for fixed time.

Figure 10. Boundary heat flux \(q_{\text{es}}\) as a function of time for various time steps with inexact data (enthalpy method)
step and future information. It is clear that the closer the sensor is to the surface, the more accurate the results are. Finally, Figures 15 and 16 demonstrate that, for bigger distance $x_1$ and fixed time step $\Delta t$, one should use a higher number of future steps in order to achieve a reasonable accuracy.

When more than one sensor internal to the domain is involved, the accuracy and stability of the solution does not change significantly. What is important is the location of the first sensor and the accuracy of its measurements.

Finally, problems with $x_1 > d/2$, zero freezing range, significant sensor error and/or cases where the front moves very fast (high Stefan number) were examined. The number of necessary iterations for convergence was increased drastically, and in some of these cases the algorithm failed to converge.
Figure 13. Boundary temperature $T_{cb}$ as a function of time for various sensor locations with inexact sensor data (enthalpy method)

Figure 14. Front position as a function of time for various sensor locations with inexact sensor data (enthalpy method)

Figure 15. Boundary heat flux $q_{cb}$ as a function of time for various future time steps with inexact sensor data (enthalpy method)
Figure 16. Front position as a function of time for various time steps with inexact sensor data (enthalpy method)

CONCLUSIONS

Front fixing and front tracking FEM techniques together with the future information method were employed to simulate two inverse solidification problems. It was shown that design problems where the interface velocity is a priori known can be treated effectively with either a front fixing or a front tracking method and a proper minimization scheme based on the future information method.

The enthalpy method was also used to work out the inverse problem of calculating the boundary flux from given thermocouple temperature measurements inside a solidifying body. This inverse problem was transformed to a form similar to an inverse heat conduction problem without phase change. New algorithms are required to analyze cases with isothermal freezing front ($\Delta T = 0$), fast freezing front motion, remote sensor locations and smaller time steps. Parameter estimation problems also remain to be addressed. For example, given temperature measurements inside a solidifying body, one should be able to calculate not only the boundary conditions but also the material property variation with temperature.

Further study of solidification design problems like those reported here can lead to the automatic control of casting processes where temperature and interface location measurements can be used to control the front motion as well as the quality of the solidifying crystals. Also further applications of the present techniques to welding and ablation processes are expected.

ACKNOWLEDGEMENTS

This work has been funded by NSF Grant CBT-8802069 to the University of Minnesota and by the Alcoa Foundation. The computing for this project is supported by the University of Minnesota Supercomputer Institute and the Cornell National Supercomputer facility, which receives major funding by the NSF and IBM Corporation, with additional support from New York State. The help of Tianhong Ouyang and Yimin Ruan in preparing some of the numerical examples is appreciated. The author would also like to acknowledge the referee’s suggestions and Dr Joshua C. Liu of Alcoa Laboratories who motivated his interest on the inverse problem B reported in this paper.
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