Thermomechanical Final State Design of Unidirectional Solidification Processes

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Abstract: This paper addresses the design of unidirectional solidification processes that result in desired final thermomechanical states. In particular, a methodology is presented for the calculation of the optimum cooling temperature history on the fixed boundary of a unidirectionally solidifying body that, at a given final process time, produces a solid shell with a uniform desired lateral residual stress distribution and a desired uniform temperature distribution. A moving FEM approach is used for the thermal part of the solidification process and an approximate incremental hypoelastic-viscoplastic model is employed in the thermomechanical analysis.

A sensitivity analysis is introduced to minimize an appropriate error norm. The effect on the solution of the process time, of the initial solution guess, and of the values of the desired uniform residual stress and temperature are examined and discussed.

INTRODUCTION

An extensive part of the literature on casting processes is devoted to the development of models for the calculation of thermal stresses and deformations in solidifying bodies. Thermal stresses are directly related to the formation of cracks in the solid shell during solidification, and thermal strains can lead to unwanted air gaps between the mould and the solid shell and distortions in final cast products. Thus, their study is very important in improving the quality of castings and their processing.

The analysis presented here is simplified by assuming a unidirectional solidification of a pure metal in a rectangular mould. The effects of fluid convection in the melt on the thermal stress development are not considered, and the interaction between the mould and the solid shell is neglected. Such interaction can lead to the formation of air gaps in the solid shell/mould interfaces, which drastically affect the heat transfer mechanisms and the traction boundary conditions on the solid shell/mould interface. The thermomechanical analysis is performed in an uncoupled fashion. First, the solution of the Stefan problem is obtained, and then, using the calculated temperature field and freezing interface location history, the deformation problem is solved in the solid shell.

There is extensive literature on Stefan problems. A review of analytical and numerical methods for their solution is given in Crank [1]. The main difficulty in Stefan problems arises from the fact that the freezing front velocity and location have to be calculated as part of the solution. The various solution techniques differ in the way they account for the motion of the solid/liquid interface. Zabaras and Ruan [2] have treated the freezing interface velocity and location as primary variables of the heat conduction analysis, and introduced a proper energy preserving calculation of the freezing front velocity in a deforming finite element analysis.

The literature on inverse Stefan solidification problems is extensive. For a typical inverse Stefan problem, it is assumed that the boundary flux conditions on the fixed mould surface are
NOMENCLATURE

- $a(T)$: thermal expansion coefficient
- $B$: matrix due to the motion of the finite element nodal points
- $C$: heat capacity matrix
- $c$: specific heat
- $E$: number of elements
- $E(T)$: temperature dependent Young's modulus
- $F$: finite element load vector
- $J$: cost functional
- $L'$: latent heat of fusion
- $L_3$: the set of square integrable functions
- $M$: number of nodes
- $\rho$: fluid melt pressure at the interface
- $P$: vector of optimization parameters
- $t$: time
- $t_f$: total processing time
- $t_{sol}$: total solidification time
- $T$: temperature
- $T_m$: melting temperature
- $\hat{T}$: desired final temperature
- $T':$ vector of computed final nodal temperatures
- $\dot{T}$: vector of desired nodal temperatures
- $u$: displacement
- $W_0$: weighting parameter
- $X$: sensitivity coefficient matrix

Greek Symbols

- $\dot{\varepsilon}$: strain rate tensor
- $\phi_i(t)$: cubic spline interpolation functions
- $\Phi$: finite element shape function
- $\lambda$: tolerance
- $\lambda(T), \mu(T)$: temperature dependent Lamé parameters
- $\rho$: density
- $\sigma$: Cauchy stress tensor
- $\sigma^*$: Cauchy stress tensor at the solid/liquid interface
- $\sigma_e$: effective stress
- $\sigma$: vector of computed final nodal stresses
- $\hat{\Sigma}$: vector of desired uniform nodal stresses
- $\hat{\Sigma}$: desired lateral residual stress distribution
- $\Omega$: optimization weighting matrix

Not known and must be determined from the temperature measurements at some interior points in the mould and/or the solidifying shell. In the inverse Stefan design problem, the material properties, initial temperature, melting temperature, the motion/location of the freezing front at all times, and the boundary flux in the solid side of the freezing interface are given. The main unknown of this design problem is the boundary flux history on the fixed mould boundary. It is known that the freezing front motion and the flux on the solid side of this front define the crystallographic growth morphology and scale of microstructures. As our preliminary research has shown, it is possible to address and solve these design solidification problems where the history of boundary cooling conditions that result in a desired crystallographic growth morphology and scale of microstructures is calculated (Zabaras et al. [3–5]). The cast structure is selected such that desired macroscopic mechanical properties of the casting are achieved. An extensive review of methods for the solution of such Inverse and Design Stefan problems is given in Zabaras et al. [3]. Inverse ill-posed problems are characterized by the fact that their solutions are unstable with respect to small changes in the given/desired data and not always unique. Minimization techniques in both finite and infinite dimensional function spaces have been employed for their solution (Zabaras and Kang [5]). References [3,4] use a time marching scheme with appropriate regularization in space as well as time smoothing, while Reference [5] employs the adjoint method and gradient techniques of optimization.

The deformation part of the solidification problem is more complicated than the heat transfer. A proper model of deformations should account for the fact that the solid region grows with time in such a way that a material liquid particle preserves its stress state as it first solidifies. To
account for such an initial condition, the problem has to be treated as an initial boundary value problem (Zabaras et al. [6,7]). This point, first discussed by Richmond and Tien [8] and Tien and Richmond [9], was implemented in one-dimensional solidification problems by Heinlein et al. [10], in two-dimensional plane stress applications by Zabaras et al. [6], and in axially symmetric problems by Zabaras et al. [7].

With the freezing interface motion specified through a front tracking FEM heat transfer analysis, one can easily account for the mechanical initial conditions at the freezing front. Zabaras et al. [6,7] used a rate form of the principle of virtual work together with a hypoelastic-viscoplastic constitutive model to account for the isostatic stress state at the freezing interface and to calculate the thermal stress distribution during solidification. The mechanical and thermal properties were allowed to vary with temperature. Numerical simulations of the solidification of pure aluminum were performed under realistic material representation and thermomechanical boundary conditions. The effects of different boundary cooling conditions on the development of thermal stresses were examined and the obtained results have shown the direct and significant effect of the cooling boundary conditions on the values and distribution of the thermal stresses at the end of solidification.

Irregular residual stresses induced by casting always survive the stages of subsequent forming processes. Often, the release of these residual stresses brings undesirable dimensional changes. In the case of metals under heavy load, high or uneven residual stresses may attenuate the stresses and result in failure: they can cause an increased susceptibility to fatigue and stress corrosion. Therefore, it becomes necessary to control the casting process so that a desired residual stress distribution is obtained.

In the present work, a least squares methodology is proposed to obtain the optimum time history of boundary temperature that results in a desired uniform residual stress distribution at the end of the casting process. Here, the casting process includes both the solidification as well as the subsequent cooling operation that is necessary to obtain a uniform ambient temperature throughout the solid shell. A brief review of the direct thermomechanical solidification analysis is presented. Then the optimization problem is defined and the solution technique is developed in a finite dimensional function space. The time history of boundary temperature which, in a given process time, results in a desired uniform residual stress, is obtained for the solidification and subsequent cooling of a commercially pure aluminum. The effect on the solution of the process time, of the initial solution guess, and of the values of the desired uniform residual stress and temperature is examined and discussed.

GOVERNING EQUATIONS

A liquid at initial temperature \( T_L(x) \) is assumed to occupy a region \( \Omega = [0,H] \times [0,L] \) (Figure 1). At time \( t > 0 \), the boundary \( x = 0 \) is cooled down to a temperature \( T_L(t) \) lower than the fusion temperature, \( T_w \). Unidirectional solidification starts on the boundary \( x = 0 \) and proceeds upward. Let us denote the freezing front location at time \( t \) as \( h(t) \). The governing equations in the absence of heat sources are given by Crank [1] as:

\[
C_s \frac{\partial T_s(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ K_s \frac{\partial T_s(x,t)}{\partial x} \right] \quad 0 \leq t \leq t_f, \quad 0 \leq x \leq h(t) \tag{1}
\]

\[
C_L \frac{\partial T_L(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[ K_L \frac{\partial T_L(x,t)}{\partial x} \right] \quad 0 \leq t \leq t_{sol}, \quad h(t) \leq x \leq H \tag{2}
\]

\[
K_s \frac{\partial T_s(h(t),t)}{\partial x} - K_L \frac{\partial T_L(h(t),t)}{\partial x} = \varrho_c \dot{h}(t) \quad 0 \leq t \leq t_{sol} \tag{3}
\]
where \( \mathcal{L} \) is the latent heat of fusion, \( \hat{h}(t) \) is the freezing front velocity at time \( t \), \( \dot{h}(t) = dh/dt \), and Equation (3) express a heat energy balance at the freezing front (the Stefan Condition) during solidification. \( T_S(x,t) \) is the temperature at the point \( x \in [0,h(t)] \) at time \( t \in [0,t_f] \), \( T_L(x,t) \) is the temperature at \( x \in [h(t),H] \) at time \( t \in [0,t_{sol}] \), and \( \varrho, c \) and \( K \) are the density, specific heat and conductivity, respectively. Subscripts \( S \) and \( L \) are used to indicate the solid and liquid phases, respectively, and the total solidification time, \( t_{sol} \), is defined from the equation \( h(t_{sol}) = H \). A zero boundary flux (insulated boundary) is assumed for the surface \( x = H \). In summary, the Stefan problem is to find the temperature history on \([0,H] \times [0,t_{sol}] \) and the solid/liquid interface velocity and location history at \([0,t_{sol}] \). For time \( t_{sol} \leq t \leq t_f \), a heat conduction problem without phase change must be solved in the fixed region \( \Omega \). The initial temperature condition for this problem is calculated from the solution of the Stefan problem at \( t = t_{sol} \), while its boundary conditions are defined by Equations (7) and (8) for \( t_{sol} \leq t \leq t_f \).

For the deformation problem, a quasi-static stress analysis is employed and attention is given only to the solid phase. Body forces and inertia forces are neglected, leading to the simple mechanical equilibrium equations

\[
\sigma_{ij}(x,t) = 0 \quad i,j = 1,2,3 \quad \text{ (summation on } i) \quad (x,y) \in [0,h(t)] \times [0,L], \quad 0 \leq t \leq t_f
\]

where \( \sigma_{ij} \) are the Cartesian components of the Cauchy stress tensor at time \( t \). As already discussed in the introduction, the deformation of the solid shell differs from that of a fixed body in that a solidifying body develops residual stresses immediately upon solidification and is never

![Figure 1](image-url). Geometry for the unidirectional solidification problem.
in a stress free state. More specifically, the stress state at the solid/liquid interface is assumed to be purely isostatic, i.e.

\[ \sigma_{11}^s = \sigma_{22}^s = \sigma_{33}^s = -p(t) \]  
\[ \sigma_{12}^s = \sigma_{13}^s = \sigma_{23}^s = 0 \]

where \( p(t) \) is the fluid (melt) pressure at time \( t \) at the freezing interface points on \( x = h(t) \), i.e.

\[ p(t) = \varrho g(H - h(t)) \]

To correctly account for the above condition, References [6] and [7] have treated the deformation problem as an initial boundary value problem rather than as a boundary value problem. To be consistent with this statement, all governing equations except the equilibrium equations must be expressed in rate form.

Assuming small strains and rotations, the total strain rate tensor, \( \dot{\epsilon}_{ij} \), is additively decomposed into an elastic (\( \dot{\epsilon}_{ij}^e \)) a thermal (\( \dot{\epsilon}_{ij}^T \)) and an inelastic (\( \dot{\epsilon}_{ij}^n \)) part, respectively. Therefore,

\[ \dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^T + \dot{\epsilon}_{ij}^n \quad i,j = 1,2,3 \]

where in terms of the rate of displacement field \( \dot{u}_i \), \( \dot{\epsilon}_{ij} \) can be calculated as

\[ \dot{\epsilon}_{ij} = \frac{1}{2}(\dot{u}_{i,j} + \dot{u}_{j,i}) \]

To account for the initial stress behavior, a hypoelastic constitutive equation is assumed for the evolution of stress,

\[ \dot{\sigma}_{ij} = E_{ijkl}(T)\ddot{\epsilon}_{kl} \quad i,j,k,l = 1,2,3 \]

where the superimposed dot denotes a time derivative, and the temperature dependent elastic constants \( E_{ijkl}(T) \) are given as

\[ E_{ijkl}(T) = \lambda(T)\delta_{ij}\delta_{kl} + \mu(T)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \]

where \( \lambda(T) \) and \( \mu(T) \) are the temperature dependent Lamé parameters and \( \delta_{ij} \) is the Kronecker delta. Dilatational thermal strains are assumed as

\[ \dot{\epsilon}_{ij}^T(T) = \delta_{ij} \int_{T_m}^{T} a(\nu)d\nu \]

where \( a(T) \) is the temperature dependent coefficient of thermal expansion.

Finally, a viscoplastic constitutive model is needed to prescribe the inelastic deformation. Important effects such as rate sensitivity, strain hardening and recovery must be incorporated into such models. Also, they must be valid for temperatures ranging from room temperature up to the melting point of the solidifying pure metal. Several viscoplastic constitutive models fall into this category (for example, Sample and Lalli [11] or Anand’s model [12].) In the simulations reported in this paper, a simple hyperbolic-sine creep law (Tien and Richmond [9]; Heinlein et al. [10]) is used to prescribe the inelastic deformation. This constitutive law has the following form

\[ \dot{\epsilon}_{ij}^n = \frac{3}{2} Ae^{-(e/T_m)} \frac{\sinh B\vartheta}{\vartheta} s_{ij} \quad i,j = 1,2,3 \]
TABLE 1. Thermal and Mechanical Properties of Aluminum (Zabaras et al. [6]).

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K_L ) (kcal/ms·°C)</td>
<td>0.0548</td>
</tr>
<tr>
<td>( K_L ) (kcal/ms·°C)</td>
<td>0.0548</td>
</tr>
<tr>
<td>( c_s ) (kcal/kg·°C)</td>
<td>0.2526</td>
</tr>
<tr>
<td>( c_L ) (kcal/kg·°C)</td>
<td>0.2526</td>
</tr>
<tr>
<td>( L ) (kcal/kg)</td>
<td>94.44</td>
</tr>
<tr>
<td>( q ) (kg/m³)</td>
<td>2650</td>
</tr>
<tr>
<td>( T_m ) (°C)</td>
<td>660</td>
</tr>
<tr>
<td>( T_w ) (°C)</td>
<td>660</td>
</tr>
</tbody>
</table>

Poisson's ratio \( \nu \) = 0.37

Young's modulus* \( E(0^\circ C) = 6.93 \times 10^4 \) MPa, \( E(660^\circ C) = 4.0458 \times 10^4 \) MPa

Coefficients of constitutive law [Equation (6)]

\[
A = 0.382 \times 10^{11} \text{ sec}^{-1}, \quad B = 0.0371 \text{ l/MPa}, \quad C = 18.849^\circ \text{K}, \quad n = 3.84
\]

Thermal expansion coefficient \( a(T) \)**

\[
a(25^\circ C) = 23.19 \times 10^{-6} \text{ m/m·°C}, \quad a(300^\circ C) = 27.86 \times 10^{-6} \text{ m/m·°C}
\]

\[
a(400^\circ C) = 30.23 \times 10^{-6} \text{ m/m·°C}, \quad a(660^\circ C) = 38.555 \times 10^{-6} \text{ m/m·°C}
\]

*The variation of \( E(T) \) is assumed to be linear within the temperature interval 0–660°C.

**The variation of \( a(T) \) is assumed to be piecewise linear within the temperature intervals 25–300°C, 300–400°C and 400–660°C.

where \( A, B \) and \( C \) are material constants given in Table 1 for pure aluminum, \( \bar{\sigma} \) is the effective stress defined as \( \bar{\sigma} = \sqrt{(3/2)\sigma_{ij} \delta_{ij}} \), and \( \sigma_{ij} \) are deviatoric stresses defined as \( \sigma_{ij} = \sigma_{ij} - (1/3) \sigma_{kk} \delta_{ij} \). The temperature \( T \) is in degrees Celsius and \( C \) is in degrees Kelvin. The complete deformation problem is defined by Equations (9)–(16) together with proper traction and/or displacement boundary conditions, as shown in Figure 1. This problem is coupled with the heat transfer problem described earlier. The cooling boundary conditions are applied directly at \( x = 0 \), which here is assumed to be a fixed boundary at all times.

In order to derive a semi-analytical solution for the stress problem, Richmond and coworkers (Heinlein et al. [10]), taking into account the one-dimensional nature of the stress field, assumed that

\[
\sigma_i(x,t) = \sigma_i(x,t) = -p(t) + \tau(x,t), \quad \sigma_i(x,t) = -p(t)
\]

\[
\varepsilon_i(x,t) = \varepsilon_i(x,t) = 0
\]

where, in general, the stress \( \tau(x,t) \) is tensile. Instead of the constitutive model given by Equation (13), they assumed a model of the form

\[
\sigma_i(x,t) = E_{ijkl}(T)\varepsilon_i^{(k)} + \sigma_i^{(t*)}(t*)
\]

or equivalently in the form

\[
\dot{\sigma}_{ij} = E_{ijkl}(T)\dot{\varepsilon}_i^{(k)} + \dot{\sigma}_{ijkl}(T)\dot{\varepsilon}_i^{(k)}
\]

where \( \sigma_i^{(t*)}(t*) \) is an appropriate initial stress to be evaluated such that \( \tau(x,t*) = 0 \), where \( t* \) is the time at which the freezing front arrives at the location \( x \). They referred to the constitutive model (18a) as representing "a departure from the classical theory of elasticity," but no direct connection with hypoelasticity [Equation (13)] was made. From \( \dot{\varepsilon}_i = 0 \) and using Equations (11), (17a), and (18a), one can finally show that

\[
\frac{\tau(x,t)}{E(T)} = \frac{1}{1 - \nu} \left[ \frac{1 - 2\nu}{E(T)} p(t) - \frac{1 - 2\nu}{E(T_\omega)} p(t*) - \varepsilon_i^{(k)} - \varepsilon_i^{(k)} \right]
\]
where the second term in the right-hand side resulted from the initial stress \(\sigma_0(t^*)\) term in Equation (18a), and it was added to guarantee that \(\tau(x,t^*) = 0\).

In previous work of the senior author and colleagues [6,7], the hypoplastic model was implemented [Equation (18b)] without the second term in the right-hand side of the equation. The expression for the stress \(\tau(x,t)\) takes a more complicated form than that given by Equation (19). To simplify the calculations performed here, the approximation (19) for the lateral stress \(\tau(x,t)\) will be used heretofore. It was shown that this is an excellent approximation of the hypoplastic model, assuming that the hydrostatic pressure remains small [13]. With this approximation, the viscoplastic model given by Equation (16) can be simplified as follows:

\[
\dot{\varepsilon}^\tau = \frac{A}{2} e^{-(C_1 T + 273)} \frac{\sinh B \dot{\sigma}}{\dot{\sigma}} \tau(x,t), \quad \dot{\sigma} = |\tau(x,t)|
\]

Upon completion of the solidification process \(t_{sd} \leq t \leq t_f\), a modified version of Equation (19) is used for the calculation of \(\tau(x,t)\). Specifically, an elastic model is used instead of a hypoplastic one and the second term on the right-hand side of Equation (19) is absent. The first term on the right-hand side of the same equation is zero \((p(t) = 0\), for \(t_{sd} \leq t \leq t_f\).

**DEFINITION OF AN INVERSE FINAL STATE DESIGN PROBLEM**

Different criteria of optimality of a solidification process are now stated. In particular, of major concern are the criteria of obtaining residual stresses which are as uniform as possible, minimizing the maximum (usually tensile) stresses at the early stage of solidification or minimizing the residual distortions. In most of the above cases, one could consider as a major independent variable the time history of the applied thermal cooling boundary conditions at \(x = 0\). These optimization problems fall in the general category of the so-called inverse retrospective optimum design solidification problems.

In such problems, the time history of boundary cooling is needed that will lead to an optimum result (for example, minimum residual stresses) at the end of the process. In this work, the end of the casting process, time \(t_f\), is defined not as the time \(t_{sd}\) at which the last liquid solidifies \([h(t_{sd}) = H]\), but as the time at which some additional cooling has occurred and a uniform desired ambient temperature has been obtained throughout the solid shell. In this work, we assume that the boundary temperature history \(T_b(t)\) is not given a priori and that it must be found as a control function—solution of a proper optimization problem.

Optimal control heat conduction problems have been investigated in the past by several workers [14,15]. Meric [16,17] has investigated some terminal control heat conduction problems. In particular, he designed optimal heating by controlling the ambient temperature, such that at a specified final time, \(t_f\), the final temperature distribution approaches a desired uniform temperature as close as possible and with a minimum energy expense.

Here, of particular interest is the problem of obtaining, at a given final process time, \(t_f\), a residual stress distribution as close as possible to a desired stress distribution \(\tilde{\tau}(x)\) and a final temperature distribution equal to \(\tilde{T}\) (ambient temperature). It is required to obtain the cooling history, \(T_b(x)\), that at time \(t_f\) leads to the above desired final state. In the examples considered in this paper, a uniform residual stress distribution is assumed \([\tau(x) = \text{constant}]\). However, in multidimensional solidification problems, uniformity of the residual stresses cannot be achieved. As such, in the notation of this paper, we will preserve the spatial dependence of \(\tau(x)\).

Considering the desired final temperature as “the desired terminal state” and the deviation of the calculated final lateral residual stress distribution from the desired one as the “expenditure,” one could pose the problem as a *terminal control heat conduction problem* with a minimum “residual stress expenditure.” In this sense, the problem can be defined as follows:

Find the optimal time history of boundary temperature \(T_b^*(t)\) such that

\[
(T_b^*(t)) \leq (T_b(t)), \quad T_b(t) \in L_1(0,t_f)
\]
where
\[ \langle T_s(t) \rangle = \frac{1}{2} \| \mathbf{z}(x,t_f; T_s(t)) - \mathbf{\hat{z}}(x) \|_{2_{L^1(0,H)}} \]  
(21b)

with the constraint
\[ T(x,t_f; T_s(t)) = \mathbf{\hat{T}} \]  
(21c)

where the normalized quantities \( \mathbf{z} \), \( \mathbf{\hat{z}} \), \( \mathbf{T} \), and \( \mathbf{\hat{T}} \) are defined as
\[ \mathbf{z} = B \tau, \quad \mathbf{\hat{z}}(x) = B \mathbf{\hat{x}}(x) \]
(21d)

\[ \mathbf{T} = (T - \mathbf{\hat{T}})/(T_w - \mathbf{\hat{T}}) \]  
and \( \mathbf{\hat{T}} = 0 \)

where \( B \) is the material constant used in the inelastic constitutive law (see Table 1). \( L_2([0,H]) \) is the set of square integrable functions in the space domain \([0,H]\) and for any function \( f(x) \in L_2([0,H]) \), the norm above is defined as
\[ \| f(x) \|_{2_{L^1(0,H)}} = \int_0^H f^2(x)dx \]  
(22)

The notation for the final states \( r(x,t_f; T_s(t)) \) and \( T(x,t_f; T_s(t)) \) is used to emphasize the fact that both are functions of the boundary temperature history, \( T_s(t) \), and that \( t_f \) is given. An observation must be made for the problem defined by Equations (21a)–(21d). Each boundary temperature history \( T_s(t) \) provides (via the direct heat conduction problem) the temperature distribution \( T(x,t; T_s(t)) \) everywhere in the domain \( \Omega \) and at any time \( t, 0 \leq t \leq t_f \). The “cost” of each solution \( T_s(t) \), defined by Equation (21b), is obtained via the solution of a direct thermo-mechanical problem (a non-heat conduction problem) with a given temperature field. More than one function \([T_s(t)]\) exists that satisfies the constraint (21c). From these functions, we are interested in selecting the one that minimizes the “residual lateral stress expenditure” defined by Equation (21b). Considering the design aspect of the proposed problem, uniqueness of the solution is not an important issue and any physically admissible solution will suffice. For physical admissibility and to restrict the number of possible solutions, a parameterization of the function \( T_s(t) \) is considered in an appropriately defined finite dimensional functional space.

From an implementation point of view, it is advisable to treat both desired criteria as parts of the objective function, and thus modify the definition of the above problem as follows:

Find the optimal time history of boundary temperature \( T^*_s(t) \) such that
\[ J(T^*_s(t)) \leq J(T_s(t)), \quad T_s(t) \in L_2(0,t_f) \]  
(23)

where
\[ J(T_s(t)) = \frac{1}{2} \| \omega_1(x)(\mathbf{z}(x,t_f; T_s(t)) - \mathbf{\hat{z}}(x)) \|_{2_{L^1(0,H)}} \]
\[ + \frac{1}{2} \| \omega_2(x)(\mathbf{T}(x,t_f; T_s(t)) - \mathbf{\hat{T}}) \|_{2_{L^1(0,H)}} \]  
(24)

\( \omega_1(x) \) and \( \omega_2(x) \) are positive weight functions that are introduced for the calculation of weak solutions that satisfy the two desired final state constraints only in some relative manner.
DEVELOPMENT OF THE METHOD

Solution of the Direct Stefan Problem

To demonstrate the method, let us 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 freezing interface. The shape functions are assumed to implicitly depend on time through the time dependence of the nodal coordinates. Let $T^*_j(t)$ be the nodal temperatures, $\Phi^*_i(x,t)$ the time dependent element shape functions, $i = 1,2,\ldots,M^*$, where $M^*$ is the number of nodes in the element $e$ (the subscript $S$ indicating solid phase is dropped for notational convenience). One can assume an isoparametric transformation of the real space $x$ to the time independent space $\xi$, with $-1 \leq \xi \leq +1$ and use the familiar isoparametric shape functions $\Phi^*_i(\xi)$. Assuming that the solid phase is divided into $E$ elements ($e = 1,E$) with $M$ nodes, one can show that at each time $t$, the weak Galerkin formulation for Equation (1) takes the following final discretized form:

$$
C_{ij} \frac{dT^*_j}{dt} + (B_{ij} + K_{ij})T^*_j = F_i \quad i = 1,M, \quad j = 1,M \quad \text{(sum on } j) \quad (25)
$$

where

$$
B_{ij} = \sum_e B^*_{ij} = -\sum_e \int_{\Omega_e} e^* \frac{dx}{dt}(x,t)\Phi^*_i(x,t) \frac{\partial \Phi^*_j(x,t)}{\partial x} \, dx
$$

(26)

The expressions for $[K]$, $[C]$ and $[F]$ are of the same form as for a non-moving finite element methodology. The matrix $[B]$ accounts for the artificial motion of the nodes [2]. Here, the finite element nodes are set such that a uniform mesh is always preserved. The Crank-Nicolson time marching scheme is used to iteratively integrate Equation (25). The involved matrices are functions of $h(t)$ and $h(t)$. This freezing front velocity is iteratively calculated from the Stefan condition [Equation (3)]. The required freezing front flux discontinuity is evaluated from the time-discretized version of Equation (25) (combined version for both solid and liquid phases) at the freezing interface nodes where the isothermal condition of Equation (4) is applicable (compatibility conditions). This iterative process is accurate, easy to implement and has been shown to preserve energy [2].

Direct Calculation of the Lateral Stress $\tau(x,t)$

Equation (19) has been solved in an iterative time stepping process. The non-linear strain, $e^*_s$, is calculated by an explicit numerical integration of Equation (20). This integration is implemented for each mesh point using the predicted stresses and already calculated temperature values at that point. The time of arrival of the freezing front at each mesh point is calculated by numerical interpolation of the freezing front locations calculated from the direct Stefan problem. The time step used in the integration of the constitutive model is usually much smaller than the one used in the heat transfer analysis. The required temperatures and freezing interface locations at these steps can be calculated from the ones obtained in the heat transfer analysis via a linear interpolation. Also note that, even though the mesh used in the stress analysis coincides with that used in the solid phase of the heat transfer analysis, a Lagrangian fixed grid approach was used for the integration of the constitutive model.

Algorithm for the Inverse Final State Design Problem

To solve the optimization problem in a finite dimensional function space, an $N$th dimensional approximation of $T^*_s(t)$ is introduced:
where $N$ is the number of a priori defined basis functions, $\phi_i(t) \in V_N(0,t_f)$, and $V_N(0,t_f)$ is the approximation function space. Here, cubic spline interpolation functions $\phi_i(t)$ are used and $p_i = T_i(t_i), i = 1,N$, where $t_i = t_f(i - 1)/(N - 1)$ are equally spaced nodes on the time interval $[0,t_f]$.

A discretized form of the functional (24) can now be written as follows: find coefficients $p_j$, $j = 1, \ldots,N$, such that

\[
J(p_j) = \frac{1}{2} \sum_{i=1}^{M} W_{si}[\tau(x_i,t_f; p_1,p_2,\ldots,p_N) - \hat{\tau}(x_i)]^2
+ \frac{1}{2} \sum_{i=1}^{M} W_{si}[T(x_i,t_f; p_1,p_2,\ldots,p_N) - \hat{T}]^2
\]

is minimized for given $\hat{\tau}(x_i)$ and $\hat{T}$, where $W_{si}$ and $W_{zi}$ are the given weighting parameters depending on the physical interpretation of the optimization problem and $x_i$ are the nodes on the uniform space discretization ($x_i = H(i - 1)/(M - 1), i = 1,2,\ldots,M$). Note that $W_{si}$ and $W_{zi}$ are functions of the weights $\omega_i(x_i)$ and $\omega_i(x_i)$ defined earlier, the space discretization, the integration scheme involved in the $L_2$-norm calculation of Equation (24) and of the material parameters used to non-dimensionalize residual stress or temperature, respectively [Equation (21c)]. The selection of the weighting parameters $W_{si}$ and $W_{zi}$ emphasizes the relative importance of the two terms in the above cost functional, $J$.

Assuming an iterative process for the calculation of the parameter vector $p^{**} = [p_1^{**}, p_2^{**}, \ldots,p_N^{**}]$, the above cost functional at the $k + 1$th iteration can be represented in a matrix form as:

\[
J(p^{**}) = \frac{1}{2} (\Sigma(p^{**}) - \hat{\Sigma})^T \Omega_1 (\Sigma(p^{**}) - \hat{\Sigma}) + \frac{1}{2} (\Phi(p^{**}) - \hat{\Phi})^T \Omega_2 (\Phi(p^{**}) - \hat{\Phi})
\]

where the vectors $\Sigma, \hat{\Sigma}, \Phi$, and $\Phi$ represent computed final stress distribution, desired uniform stress distribution, computed final temperature distribution, and desired temperature distribution, respectively, defined as

\[
(\Sigma)_i = \tau(x_i,t_f; p^{**}), \quad (\hat{\Sigma})_i = \hat{\tau}(x_i), \quad (\Phi)_i = T(x_i,t_f; p^{**}), \quad \text{and} \quad (\hat{\Phi}) = \hat{T}
\]

$\Omega_1$ and $\Omega_2$ are optimization weighting matrices defined as

\[
\Omega_1 = \text{diag} \left( W_{s1}, W_{s2}, \ldots, W_{sN} \right)
\]

\[
\Omega_2 = \text{diag} \left( W_{z1}, W_{z2}, \ldots, W_{zN} \right)
\]

A linearization of the final states with respect to the unknown parameters gives

\[
\Sigma(p^{**}) = \Sigma(p^*) + X_1|_{p=p^*} \Delta p^*
\]

\[
\Phi(p^{**}) = \Phi(p^*) + X_1|_{p=p^*} \Delta p^*
\]
\[ \Delta p^* = p^{*+1} - p^* \] and the sensitivity coefficient matrices \( X_1 |_{\rho p^*} \) and \( X_2 |_{\rho p^*} \) are defined as:

\[
(X_1 |_{\rho p^*})_{ij} = \frac{\partial \tau(x_i, t_j; \rho p^*)}{\partial \rho p_i} \bigg|_{\rho p^*} \quad i = 1, \ldots, M, \quad j = 1, \ldots, N \tag{34a}
\]

\[
(X_2 |_{\rho p^*})_{ij} = \frac{\partial T(x_i, t_j; \rho p^*)}{\partial \rho p_i} \bigg|_{\rho p^*} \quad i = 1, \ldots, M, \quad j = 1, \ldots, N \tag{34b}
\]

The sensitivity coefficient matrices are computed using finite difference approximations similar to those employed in Reference [4]. For example, the calculation of \( X_1 \), has as follows:

\[
(X_1 |_{\rho p^*})_{ij} = \frac{\tau(x_i, t_j; p^*_1, \ldots, p^*_j(1 + \epsilon), \ldots, p^*_j) - \tau(x_i, t_j; p^*_1, \ldots, p^*_j, \ldots, p^*_j)}{\epsilon p^*_j} \tag{35}
\]

\[ i = 1, \ldots, M, \quad j = 1, \ldots, N \]

where here, \( \epsilon = 0.001 \).

Substituting Equations (32) and (33) into Equation (29) and differentiating it with respect to \( \Delta p^* \) results in the following system of algebraic equations:

\[
[X_1^T(p^*) \Omega_1 X_1(p^*) + X_1^T(p^*) \Omega_2 X_2(p^*)] \Delta p^* = X_1^T(p^*) \Omega_1 (\Theta - \Delta(p^*)) + X_1^T(p^*) \Omega_2 (\hat{T} - T(p^*)) \tag{36}
\]

In summary, the algorithm is given as follows.

Assume that all the parameters, \( p^* \), are known at the \( k \)th iteration.

1. Using \( p^* \), compute the final temperature distribution \( T(x_i, t_j; p^*) \) via a direct heat transfer analysis and the residual stress distribution \( \tau(x_i, t_j; p^*) \) by solving the direct thermomechanical problem. The calculation of \( T(x_i, t_j; p^*) \) requires the solution of a Stefan problem for \( 0 \leq t \leq t_{al} \), and then the solution of a heat conduction problem for \( t_{al} \leq t \leq t_f \). The calculation of \( \tau(x_i, t_j; p^*) \) requires the integration of Equation (20) and the evaluation of the right-hand side of Equation (19).

2. Construct the sensitivity coefficient matrices \( X_1 \) and \( X_2 \) using finite difference approximations. (This step requires the solution of \( N \) additional heat transfer and thermomechanical direct problems.)

3. Solve the system of Equation (36) to obtain \( \Delta p^* \) and update parameters: \( p^{*+1} = p^* + \Delta p^* \).

4. Check for convergence.

If \( \| \Delta p^* \| < \lambda p^* \), where \( \lambda \) is a given tolerance, convergence has been achieved and the algorithm stops. Otherwise, \( k = k + 1 \) and we repeat the calculations starting from step 1.

In the numerical results reported later in this paper, instead of the tolerance technique of step 4 above, the algorithm was repeated for a number of iterations until \( \| \Delta p^* \| / p^* \) achieved a minimum or remained in a flat plateau.

**NUMERICAL RESULTS**

The problem we are interested in is the solidification and subsequent cooling of a pure aluminum in a rectangular mould whose geometry is shown in Figure 1 (\( L = 0.01 \) m, \( H = 0.1 \) m). As mentioned earlier, the problem is unidirectional in nature. The boundary temperature history \( T_b(t) \) is uniformly applied at \( x = 0 \) and is the main unknown to be estimated from the optimization problem. The thermomechanical properties of pure aluminum are given in Table 1.
For the direct transient thermal analysis using the moving finite element method [2], 40 linear elements were used with time step $\Delta t = 0.2$. For the direct thermomechanical analysis, a direct iteration scheme is used to integrate the hyperbolic-sine constitutive equation with time step $\Delta t = 0.005$.

The unknown boundary temperature history is parameterized using a cubic spline approximation with pieces over six equal intervals within the time interval $(0, t_f)$. Since initial slope (at $x = 0$) of the cubic spline approximation cannot be fixed, it is obtained using a natural spline with zero second derivative on that boundary [18]. Initial and final boundary temperatures, $T_0(0)$ and $T_0(t_f)$, are considered equal to the melting and desired ambient temperatures, $T_m$ and $\hat{T}$, respectively. In other words, we consider $N = 7$ and that for all problems and all iterations $k$, $p_j^i = T_m = T_0$ and $p_j^f = \hat{T}$. The main parameters to be estimated are then $p_j^i$, $j = 2, \ldots, 6$.

In the following examples, the final time, $t_f$, has been selected as 300, 360, and 420 seconds. These $t_f$ values were obtained by solving several direct problems with initial design cooling conditions defined from Equation (27) with certain choices of the $p_j$s that are given later in this section. These initial designs were used in the numerical algorithm as the initial ($k = 0$) guess solution. For all the simulations, the weighting parameters, $W_1$, are assumed to vary in space and $W_2$, is assumed constant. More specifically, $W_1$, through $W_4$, were varied linearly from 2.0 to 3.0, and $W_5$ through $W_7$, were equal to $W_1$, whereas $W_8 = W_9 = 1.0$. This selection of $W_i$, is important for obtaining a reasonable solution, especially considering the relatively high tensile stresses that are induced during solidification near $x = 0$ (Zabaras and Richmond [13]).

Figure 2 shows the time histories of boundary temperature obtained at several stages of iteration with $t_i = 420$ secs, $\hat{T}(x) = 0$ MPa and $\hat{T} = 250^\circ C$. The initial design solution was selected as $\{p_1^i, p_2^i, p_3^i, p_4^i, p_5^i\} = \{405^\circ C, 325^\circ C, 285^\circ C, 265^\circ C, 255^\circ C\}$. The optimum solution, shown in Figure 2, indicates that fairly rapid cooling is required for the solidification process, followed by a slow cooling to a temperature below the desired ambient temperature, and eventually slow heating up to the ambient temperature. The solidification time, $t_{so}$, was 132.6 seconds for the initial guess and 124.0 seconds for the optimum solution.

The obtained final residual stress distribution in conjunction with the obtained optimal boundary temperature history of Figure 2 is shown in Figure 3. It is clear that the magnitude of the residual stress is much smaller than the one which results from the initial design, and that in the $L_1$ norm sense, a uniformity of the residual stress distribution is achieved by applying the optimal cooling history. It should be mentioned that, for a given material and mould geometry, one cannot choose arbitrarily the desired residual stress distribution, $(\tau(x), \text{the desired ambient temperature } \hat{T}$, and the total process time $t_f$. Such arbitrary selection generally results in a non-unique solution or in a solution that is physically unrealistic. The required compatibility condi-

![Figure 2](image-url)
tions between the given and desired data have not been investigated thoroughly. However, the initial design solutions were used as the reference conditions around which one is looking for an optimum solution.

Figure 4 shows the final temperature distribution, $T(x,t_f)$, that results from the optimum solution shown in Figure 2; an almost uniform temperature distribution close to the ambient temperature was obtained. One of the biggest reasons for distortion in casting processes is the temperature difference in different areas of a body and therefore, uniform temperature distribution at the end of the process is essential to prevent dimensional changes [19]. In this respect, the term $\| T(x,t_f; T_0(t)) - \bar{T} \|_2^2(x_{(0,M)})$ was quite successfully used in this example and its minimization is a necessary criterion for minimizing residual distortions even in more complicated cases. Minimizing thermal stresses at a stage where the temperature field is not uniform can also be an important problem, assuming that one is interested in failure of castings and in the control of the magnitude of the developed stresses.

The optimum cooling conditions are now calculated using different processing times, $t_f$. The initial design parameters for the cases $t_f = 420$ seconds, $t_f = 360$ secs, and $t_f = 300$ secs were taken as $[p^x, p^y, p^z, p^t] = \{405^\circ\text{C}, 325^\circ\text{C}, 285^\circ\text{C}, 265^\circ\text{C}, 255^\circ\text{C}\}$. Note that these parameters result in different initial design boundary temperatures as they refer to different time locations (the nodal time $t_i$ of Equation (27) refers to equally spaced intervals on $[0,t_f]$).

Figure 4. Final temperature distribution in conjunction with the obtained optimal boundary temperature shown in Figure 2 ($\bar{T}(x) = 0$ MPa, $\bar{T} = 250^\circ\text{C}$, $t_i = 420$ secs).
The effects of final time on the optimal cooling history are shown in Figure 5. These optimal solutions for \( t_f = 300, 360, \) and 420 seconds were achieved with 8, 10, and 15 iterations, respectively. The obtained tolerances at these iteration levels were 3.55\%, 0.569\% and 1.69\%, respectively. As final time \( t_f \) decreases, the cooling rate in the early stages of the solidification process increases. For \( t_f = 420 \) sec, initial cooling occurs slower and a smaller amount of undercooling is required, whereas for \( t_f = 300 \) sec, the initial cooling occurs very rapidly and a significant undercooling is required to achieve the uniform residual stress and temperature distribution. Figure 6 shows the residual stress and temperature distributions at the end of the solidification \( (t = t_{\text{eq}}) \) for the optimum conditions calculated above. For the case of \( t_f = 300 \) sec \( (t_{\text{eq}} = 119.6 \) sec), the residual stress varies from 9 to 0 MPa, while the temperature varies from 300 to 660°C. It is clearly indicated that subsequent cooling is required after solidification processing. This figure also indicates that the magnitude of the residual stress at \( x = 0 \) decreases as solidification time increases.

From Figures 5 and 6, it is fair to conclude that in general, as \( t_f \) decreases, to achieve an optimum solution, \( t_{\text{eq}} \) must decrease and the amount of undercooling should increase. Note that as \( t_f \) goes to infinity, the problem becomes highly unrealistic since the residual stresses approach zero without any special provision. In this sense, the requirement of \( t_f \) having finite values around the process time of an initial design is essential.
Figure 7. Residual stress distribution based on the optimum solutions of Figure 5 calculated at different processing times $t_r$. $\hat{\tau}(x) = 0 \text{ MPa}, \hat{T} = 250^\circ\text{C}$.

Figure 7 shows the residual stresses obtained for the different final times ($t_f$) cases in conjunction with Figures 5 and 6. The amount of deviation of these stresses from the desired final residual stress value, $\hat{\tau}(x) = 0 \text{ MPa}$, decreases as $t_f$ increases. However, as we already mentioned, the goal of the present work is to obtain the optimum cooling history that results in a uniform residual stress for a given processing time rather than at infinite time.

Figure 8 shows the effect of initial guesses on the final solution. For both cases, $t_f = 420$ secs. For the first initial design (case 1), $\{p_1^1, p_2^1, p_3^1, p_4^1, p_5^1\} = \{405^\circ\text{C}, 325^\circ\text{C}, 285^\circ\text{C}, 265^\circ\text{C}, 255^\circ\text{C}\}$, while for the second initial design (case 2), $\{p_1^2, p_2^2, p_3^2, p_4^2, p_5^2\} = \{365^\circ\text{C}, 305^\circ\text{C}, 275^\circ\text{C}, 260^\circ\text{C}, 253^\circ\text{C}\}$. The algorithm converges in 10 iteration steps with initial guess close to the converged optimal solution (case 2), whereas it converges in 15 iteration steps with initial guess a little further from the converged solution (case 1). The obtained tolerances at these iterations were 1.69% for case 1, and 1.865% for case 2. It should be noted that both converged solutions are very close to each other, and give more or less identical residual stresses, as shown in Figure 9. Final temperature distributions obtained from the different initial guesses are also identical, but are not shown here.

From the above examples, one cannot claim the uniqueness of the optimal boundary cooling history. A totally arbitrary initial guess may result in a different optimal solution which, however, may be physically unrealistic and away from any acceptable design practice. One way of
Figure 9. Residual stress distribution based on the optimum solutions of Figure 8 that were calculated using different initial guesses.

achieving a unique solution is to constrain the range of cooling history such that an arbitrary initial guess may not be used. This type of constraint may physically be motivated based on the extremes of the cooling conditions that can be achieved in practice via the available means (for example, via water spraying). A uniqueness of the solution may also be achieved by including the final time to the cost functional of the present formulation. Analysis of such minimum time solidification problems with a desired final state will be reported in a later publication.

Finally, the authors previously reported that a desired cast structure can be obtained by controlling the liquid/solid interface heat flux and front velocity [5]. In the present work, in addition to optimizing the final state, one could restrain the unknown boundary temperature such that a desired cast structure is obtained. This and similar constrained optimization problems that can guarantee uniqueness of the history of boundary cooling are the subject of ongoing research.

CONCLUSIONS

A methodology has been presented for the calculation of the optimum time history of boundary temperature that results in a residual stress distribution that is as uniform as possible, while the final temperature distribution approaches a desired ambient temperature. A finite dimensional unconstrained optimization technique utilizing sensitivity analysis was used. The problem was solved for different final times, residual stress distributions, and initial design solutions. The obtained optimum solutions indicate that a fairly rapid cooling is required for the solidification process, followed by a slow cooling to a temperature below ambient temperature, and eventually, a slow heating up to the ambient temperature.

It is a well-known fact that fast cooling in the early stages of the solidification process results in very high values of lateral stresses, which saturate towards the end of the solidification process [13]. Since the purpose of this work was to obtain a desired uniform residual stress distribution at the end of the casting process, the minimization of the maximum thermal stress occurring during the process was not included in the present formulation. It will be desirable to extend the present work and calculate the optimum cooling conditions that result in the minimization of the maximum tensile stress that is developed close to the mould wall.

In multidimensional problems, one might like to minimize the $L_2$ (in the whole body) norm of the difference between the critical residual stress $\sigma$ and the maximum value of $\sigma$ over the body, i.e., make the variation of the residual stresses of interest as uniform as possible. Eventually, appropriate failure criteria must be developed and the cooling boundary conditions that do not violate such criteria could be calculated (development of appropriate "casting limit diagrams").
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