A LEAST-SQUARES FRONT-TRACKING FINITE ELEMENT METHOD ANALYSIS OF PHASE CHANGE WITH NATURAL CONVECTION

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SUMMARY

This paper focuses on the numerical modelling of phase-change processes with natural convection. In particular, two-dimensional solidification and melting problems are studied for pure metals using an energy preserving deforming finite element model. The transient Navier–Stokes equations for incompressible fluid flow are solved simultaneously with the transient heat flow equations and the Stefan condition. A least-squares variational finite element method formulation is implemented for both the heat flow and fluid flow equations. The Boussinesq approximation is used to generate the bulk fluid motion in the melt. The mesh motion and mesh generation schemes are performed dynamically using a transfinite mapping. The consistent penalty method is used for modelling incompressibility. The effect of natural convection on the solid/liquid interface motion, the solidification rate and the temperature gradients is found to be important. The proposed method does not possess some of the false diffusion problems associated with the standard Galerkin formulations and it is shown to produce accurate numerical solutions for convection dominated phase-change problems.

INTRODUCTION

Melt flow during solidification affects the morphology of the solid/liquid interface, the solidification rate and the temperature distribution. Controlling the heat transfer and fluid flow patterns is important if control of the casting quality and production time is to be achieved. Here, the bulk fluid motion is considered to be originated from temperature gradients in the presence of gravity (natural convection). ¹

Several analytical attempts have been made to solve Stefan problems which assume no convection. Direct numerical methods in solving transient heat conduction problems with phase change have taken two basic directions; the fixed domain method and the front-tracking method. The majority of fixed domain methods use an enthalpy formulation, which incorporates both the sensible and latent heats into a new form of the governing heat flow equation and eliminates the need for explicitly tracking the location of the solid/liquid interface.²–⁴ In these techniques, the freezing interface location and velocity are calculated as part of a post-processing operation. Another fixed domain method which has not received much attention is the discontinuous element method.⁵ Here, the interface cuts each finite element it lies over into two adjacent sub-elements. The necessary integrations are performed separately over each sub-element.

Front-tracking methods treat the interface velocity and position as main explicit unknowns of the phase-change problem. When solving the energy equations with the Stefan condition, the interface motion is calculated as part of the solution. With the front motion known, the solid and
liquid domains are then adjusted to the new interface position for every time step. Both fixed mesh (different for each time step) and deforming mesh approaches can be used for numerical simulation. Transformed-grid techniques are also available where the freezing front is fixed in space and time with an appropriate co-ordinate system transformation. Fixed mesh front-tracking approaches can be found in References 6 and 7. Deforming/moving finite element methods for moving boundary-value problems are given in References 8–12.

One of the first significant investigations of phase change with natural convection was that of Sparrow et al. They solved an axially symmetric solidification problem using an implicit finite difference method and the solid/liquid interface was immobilized via a Landau transformation. For each time period, using the transformed-grid solution domain, they solved the appropriate conservation equations and from that they determined the new interface position. With a similar Landau transformation, Ramachandran et al. solved a solidification problem with natural convection but used an alternating direction implicit finite difference technique with successive over relaxation.

Finite element methods for natural convection problems were developed afterwards. In particular Marshall et al. and Strada and Heinrich developed a finite element method that computed heat transfer rates for steady-state natural convection in a rectangular enclosure with high Rayleigh numbers. Solidification problems with melt convection using a front-tracking finite element method were first analysed by O'Neill and Albert. They only concentrated on natural convection in porous media though. About the same time, Yoo and Rubinsky developed a front tracking, fixed mesh, penalty finite element method with primitive fluid variables. The conservation equations were solved independently in the solid and liquid domains. A special weak form of the Stefan condition was used to calculate the interface motion. More recent investigations of phase-change problems with natural convection have focused on using finite differences techniques with fixed-grid enthalpy methods, or front-tracking transformed-grid techniques.

In this paper, a least-squares finite element method is used for solving the phase-change problem. The resulting variational form is similar to that of Petrov–Galerkin formulations and at high convection rates does not possess some of the inaccuracies associated with false diffusion. A moving and deforming mesh similar to that of O'Neill and Albert and Zabaras and Ruan is used. The latter two approaches have been shown to conserve energy across the solid/liquid interface. Mesh deformation is controlled by using a transfinite mapping technique coupled to the moving solid/liquid interface motion. A consistent penalty method formulation is used for solving the incompressible Navier–Stokes equations. A laminar flow with no viscous energy dissipation is assumed.

This paper proceeds as follows. First the definition of the solidification problem with the governing equations, boundary and initial conditions and dimensionless quantities are given. Then, the least-squares Galerkin weak forms of the governing equations and their finite element forms are introduced. A technique for the calculation of the front velocity is also presented. The implementation of the finite element method is then discussed together with the mesh generation scheme. Finally, several numerical solidification and melting examples together with a comparative discussion of the obtained results are presented.

**PROBLEM DEFINITION**

Standard practice in heat flow theory is the use of dimensionless variables that identify the significance of competing physical mechanisms. Let \( L \) be the characteristic length, \( \rho \) the density, \( c \) the specific heat, \( K \) the conductivity, \( \alpha \) the diffusivity (\( \alpha = K/c \)), \( \mu \) the dynamic viscosity and
\( \nu \) the kinematic viscosity (\( \nu = \mu/\rho \)). Let us also denote the reference temperature with \( T_0 \) and the melting temperature with \( T_m \). The subscripts S and L are used to denote the solid and liquid phases, respectively. The characteristic scale for time is taken as \( L^2/\alpha_L \), while for velocity as \( \alpha_L/\nu \). The dimensionless temperature \( \theta \) is defined as \( \theta = (T - T_m)/(T_0 - T_m) \) where \( T \) is the actual temperature. Let us also define \( R_c = c_s/c_L \) and \( R_K = K_s/K_L \). The dynamic pressure \( \bar{p} \) is defined in terms of the pressure \( p \) as \( \bar{p} = p - \rho_0 g \bar{f} \cdot \bar{x} \), where \( \rho_0 \) is the reference density (at \( T = T_m \)), \( g \) is the gravity constant and \( \bar{f} \) is a unit vector in the direction of gravity. The dimensionless pressure is defined by dividing the dynamic pressure with the characteristic pressure \( \rho \alpha_L^2/\nu^2 \).

The key dimensionless quantities are the Stefan number (\( Ste \)), Prandtl number (\( Pr \)) and the Rayleigh number (\( Ra \)). They are defined as \( Ste = c_L(T_0 - T_m)/\eta \), \( Pr = \nu/\alpha_L \) and \( Ra = g \beta (T_0 - T_m) L^3/\nu \alpha_L \), respectively, where \( \eta \) is the latent heat and \( \beta \) the thermal expansion coefficient.

Let us now consider solidification of a pure metal. All quantities used in the remaining of the text are dimensionless, except if it is otherwise stated. At time \( t = 0 \), a liquid metal is assumed to occupy a fixed two-dimensional domain \( \Omega_0 \). At time \( t > 0 \), two time-dependent solid and liquid domains are formed in \( \Omega_0 \) and are indicated by \( \Omega_S(t) \) and \( \Omega_L(t) \), respectively (Figure 1). These regions are separated by the freezing front \( \partial \Omega(t) \).

The incompressible transient Navier–Stokes equations are utilized for modelling the flow in the melt region induced by natural convection. It is assumed that the flow is laminar and has no viscous energy dissipation. Variation in the density is assumed only to effect the buoyancy term as modelled using the Boussinesq approximation (i.e. \( \rho = \rho_0 [1 - \beta (T - T_m)] \)).

The conservation of momentum for a velocity field \( \mathbf{u} \) in \( \Omega_L(t) \) is given by

\[ \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot \tau - Pr Ra \theta_L \mathbf{f} \]

(1)

where the constitutive model for the stress is

\[ \tau = -p \mathbf{I} + 2 Pr \text{sym}(\nabla \mathbf{u}) \]

(2)

with \( \text{sym} \) denoting the symmetric part of a tensor and \( \mathbf{I} \) a second-order unit tensor.

The fluid incompressibility is stated as

\[ \nabla \cdot \mathbf{u} = 0 \]

(3a)

![Figure 1. Geometry of a solidification process](image)

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1. Boussinesq approximation
2. Prandtl number
3. Rayleigh number
4. Stefan number
5. Incompressible flow
6. Natural convection
7. Laminar flow
8. Viscous energy dissipation
or by the modified incompressibility condition\textsuperscript{24}

\[ p + \lambda (\nabla \cdot \mathbf{u}) = 0 \]  

(3b)

where the penalty number \( \lambda \gg \mu \) is assumed.

The temperature field is defined from the heat transfer equations:

\[ R_K \frac{\partial \theta_S}{\partial t} = \nabla \cdot (R_K \nabla \theta_S) \]  

(4)

\[ \frac{\partial \theta_L}{\partial t} + \mathbf{u} \cdot \nabla \theta_L = \nabla \cdot \nabla \theta_L \]  

(5)

that are applicable in the regions \( \Omega_S(t) \) and \( \Omega_L(t) \), respectively. Finally, the energy balance along the solid/liquid interface \( \partial \Omega(t) \) is expressed as

\[ R_K \frac{\partial \theta_S}{\partial n} - \frac{\partial \theta_L}{\partial n} = (Ste)^{-1} \mathbf{V} \cdot \mathbf{n} \]  

(6)

where the vector \( \mathbf{V} \) represents the solid/liquid interface velocity and \( \mathbf{n} \) is a unit vector normal to the solid/liquid interface.

The boundary conditions used for equations (1), (4) and (5) are given as follows:

\[ \mathbf{u}(x_1, x_2, t) = \mathbf{0}, \quad (x_1, x_2) \in \partial \Omega_L(t) \]  

(7a)

\[ R_K \nabla \theta_S(x_1, x_2, t) \cdot \mathbf{n} = Bi(\theta_\infty - \theta_S(x_1, x_2, t)), \quad (x_1, x_2) \in \partial \Omega_0 \]  

(7b)

\[ \theta_S(x_1, x_2, t) = \theta_L(x_1, x_2, t) = \theta_m = 0, \quad (x_1, x_2) \in \partial \Omega_L(t) \]  

(7c)

The unit vector \( \mathbf{n}_0 \) is normal to the boundary \( \partial \Omega_0 \). More general than that of equation (7b) boundary conditions can be selected as well. Here, a mixed type condition is used where \( Bi \) is the Biot number defined as \( Bi = Lh/K_L \), with \( h \) the convection coefficient and \( \theta_\infty \) the ambient temperature. In equation (7c) the melting temperature is prescribed along \( \partial \Omega_L(t) \).

The initial conditions for the problem are given as follows:

\[ \Omega_S(0) = \emptyset, \quad \Omega_L(0) = \Omega_0 \]  

(8a)

\[ \mathbf{u}(x_1, x_2, 0) = \mathbf{u}_m(x_1, x_2), \quad (x_1, x_2) \in \Omega_0 \]  

(8b)

\[ \theta_L(x_1, x_2, 0) = \theta_m(x_1, x_2), \quad (x_1, x_2) \in \Omega_0 \]  

(8c)

**FINITE ELEMENT FORMULATION**

The deforming finite element method discretization

In the solidification process both solid and liquid regions change constantly with time. A general way to model these domains is by using finite elements that can continuously move and deform. The solid and liquid regions are assumed to share the same finite element nodes on the moving front. With this way, one can allow for an accurate prescription of boundary conditions along \( \partial \Omega_L(t) \). In this paper, the deforming finite element formulation by Lynch and Gray\textsuperscript{8} and Zabaras and Ruan\textsuperscript{12} will be considered. The shape functions of each element are implicit functions of time. This time dependence results from the time dependence of the nodal coordinates of the finite elements.
Let the discrete solution in a finite element for the velocity, temperature and pressure at time \( t \) be expressed in the form

\[
\begin{align*}
    u_i(t) &= u^i(t) \Phi^a(x_1, x_2, t), \\
    \theta(t) &= \theta^a(t) \Phi^a(x_1, x_2, t), \\
    p(t) &= p^a(t) \Phi^a(x_1, x_2, t)
\end{align*}
\] (9)

where \( u^i(t), \theta^a(t) \) and \( p^a(t) \) denote the \( i \)th velocity component \((i = 1, 2), \) the temperature and pressure values, respectively, at the node \( u(\alpha = 1, 2, \ldots, N_{\text{ele}}, \) where \( N_{\text{ele}} \) is the number of nodes per element). \( \Phi^a(x_1, x_2, t) \) denotes the local shape function and from now on summation is implied on all repeated indices. The shape functions \( \Phi^a \) that are used in the pressure approximations are lower degree order than \( \Phi^a. \)

An isoparametric transformation, from the time dependent element co-ordinates to the time independent master co-ordinates, is defined for each deforming element as

\[
x_1 = X_1^a \Phi^a(\xi, \eta), \quad x_2 = X_2^a \Phi^a(\xi, \eta)
\] (10)

where \((X_1^a, X_2^a)\) denote the element nodal co-ordinates and \((\xi, \eta)\) the master co-ordinate space, with \(-1 \leq \xi, \eta \leq 1. \)

Because of the time dependent shape functions equation (9) implies

\[
\begin{align*}
    \frac{\partial u_i}{\partial t} &= \frac{du^i}{dt} \Phi^a - u^i_v \frac{\partial \Phi^a}{\partial x_j} \\
    \frac{\partial \theta}{\partial t} &= \frac{d\theta^a}{dt} \Phi^a - \theta^a_v \frac{\partial \Phi^a}{\partial x_j}
\end{align*}
\] (11a)

where \( v_j \) is a properly selected mesh velocity that is calculated from the nodal mesh velocity as

\[
v_1 = \frac{dX_1^a}{dt} \Phi^a(\xi, \eta), \quad v_2 = \frac{dX_2^a}{dt} \Phi^a(\xi, \eta)
\] (12)

Based on this mesh motion, equations (1), (4) and (5) can be modified as follows:

\[
\frac{d\mathbf{\vec{u}}}{dt} + (\nabla \mathbf{u}) \mathbf{\vec{u}} = -\mathbf{\nabla} p + \mathbf{\nabla} \cdot [2 Pr \text{sym}(\nabla \mathbf{u})] - Pr Ra \theta \mathbf{\hat{f}} \quad \text{in } \Omega_L(t)
\] (13)

\[
\sigma \frac{d\theta}{dt} + \sigma \mathbf{\vec{u}} \cdot \nabla \theta = \nabla \cdot (\kappa \nabla \theta) \quad \text{in } \Omega_0
\] (14)

where the relative motion \( \mathbf{\vec{u}} = \mathbf{u} - \mathbf{v} \) was introduced (note \( \mathbf{u} = 0 \) in \( \Omega_5(t) \), \( \sigma = R_C \) in \( \Omega_3 \) and \( \sigma = 1 \) in \( \Omega_L \), while \( \kappa = R_K \) in \( \Omega_3(t) \) and \( \kappa = 1 \) in \( \Omega_L(t) \).

The weak form of the energy equation

Let us first derive a weak form of the energy equation (14). Let us denote with \( \theta_n \) the unknown temperature field at time \( t_n, n = 1, 2, \ldots \) and let us assume that \( \theta_{n-1} \) is known. In order to calculate \( \theta_n \), we introduce the following implicit integration scheme of equation (14):^2,24,25

\[
R(\theta_n) = \sigma \frac{\theta_n - \theta_{n-1}}{\Delta t} + \sigma \mathbf{\vec{u}}_{n-1+\gamma} \cdot \nabla \theta_{n-1+\gamma} - \nabla \cdot (\kappa \nabla \theta_{n-1+\gamma})
\] (15)

where \( \gamma \) is the integration parameter, \( 0 \leq \gamma \leq 1 \) and all quantities with index \((n - 1 + \gamma)\) are referred to time \( t_{n-1+\gamma} = (1 - \gamma) t_{n-1} + \gamma t_n \) and they are calculated as follows:

\[
\begin{align*}
    \theta_{n-1+\gamma} &= (1 - \gamma) \theta_{n-1} + \gamma \theta_n \\
    \mathbf{\vec{u}}_{n-1+\gamma} &= (1 - \gamma) \mathbf{\vec{u}}_{n-1} + \gamma \mathbf{\vec{u}}_n
\end{align*}
\] (16a)

\[
\begin{align*}
    \theta_n &= \frac{1}{2} \left[ \theta_{n-1+\gamma} + \theta_{n+1+\gamma} \right] \\
    \mathbf{\vec{u}}_n &= \frac{1}{2} \left[ \mathbf{\vec{u}}_{n-1+\gamma} + \mathbf{\vec{u}}_{n+1+\gamma} \right]
\end{align*}
\] (16b)
Instead of requiring $R(\theta_e) = 0$, we will calculate the nodal values $\theta^e_\alpha (\alpha = 1, 2, \ldots, N^{ele})$ of each element from the following least-squares optimization scheme:

\[
\min \sum_{e=1}^E \int_{\Omega_e} R^2(\theta^e_\alpha) \, d\Omega_e \quad \text{for } \alpha = 1, 2, \ldots, N^{ele} \tag{17a}
\]

or equivalently:

\[
\sum_{e=1}^E \int_{\Omega_e} \frac{\partial R}{\partial \theta^e_\alpha} R(\theta^e_e) \, d\Omega_e = 0 \quad \text{for } \alpha = 1, 2, \ldots, N^{ele} \tag{17b}
\]

where $E$ is the number of elements in $\Omega_0$.

Using equations (16a) and (16b) and the interpolations given by equation (9), the above equation can be finally written as

\[
\sum_{e=1}^E \int_{\Omega_e} \left[ \Phi^e z + \gamma \Delta t \tilde{u}_{n-1+\gamma} \cdot \nabla \Phi^e z \right] R(\theta^e_e) \, d\Omega_e = 0 \tag{18}
\]

where the contribution of the diffusive term that results from the derivative $\partial R / \partial \theta^e_\alpha$ is neglected without significant loss of accuracy.²⁶,²⁷

With an integration by parts of the first diffusive term and by neglecting the second-higher order diffusive term in equation (18), the following system of algebraic equations can finally be derived for the vector $\{\theta_n\}$ of nodal temperatures:

\[
\left[ M_{n-1+\gamma} \right] \{\theta_n\} = \left\{ \frac{\theta_{n-1}}{\Delta t} \right\} + \left[ C_{n-1+\gamma} + K_{n-1+\gamma} \right] \{\theta_{n-1+\gamma}\} = \{F_{n-1+\gamma}\}
\]

or using equation (16a) in the form:

\[
\left[ \frac{M_{n-1+\gamma}}{\Delta t} + \gamma \left( C_{n-1+\gamma} + K_{n-1+\gamma} \right) \right] \{\theta_n\} = \{F_{n-1+\gamma}\} + \left[ \frac{M_{n-1+\gamma}}{\Delta t} - (1 - \gamma) \left( C_{n-1+\gamma} + K_{n-1+\gamma} \right) \right] \{\theta_{n-1}\} \tag{19}
\]

The matrices above have dimension $N^{tot} \times N^{tot}$ ($N^{tot}$ is the total number of nodes in $\Omega_0$) and they are defined as

\[
[M_{n-1+\gamma}] = \sum_{e=1}^E [M_{e-1+\gamma}], \quad [C_{n-1+\gamma}] = \sum_{e=1}^E [C_{e-1+\gamma}], \quad [K_{n-1+\gamma}] = \sum_{e=1}^E [K_{e-1+\gamma}]
\]

with nodal components given as

\[
M_{e-1+\gamma} = \int_{\Omega_e} \alpha \Phi^e \Phi^e \, d\Omega_e + \int_{\Omega_e} \sigma \gamma \Delta t \tilde{u}_{n-1+\gamma} \cdot \nabla \Phi^e \Phi^e \, d\Omega_e \tag{20a}
\]

\[
C_{e-1+\gamma} = \int_{\Omega_e} \sigma \tilde{u}_{n-1+\gamma} \cdot \nabla \Phi^e \Phi^e \, d\Omega_e + \int_{\Omega_e} \sigma \gamma \Delta t \tilde{u}_{n-1+\gamma} \cdot \nabla \Phi^e \tilde{u}_{n-1+\gamma} \cdot \nabla \Phi^e \, d\Omega_e \tag{20b}
\]

\[
K_{e-1+\gamma} = \int_{\Omega_e} \kappa \nabla \Phi^e \cdot \nabla \Phi^e \, d\Omega_e \tag{20c}
\]

where $\alpha, \beta = 1, \ldots, N^{ele}$, and the solid or liquid material properties are used depending if $\Omega_e \subseteq \Omega_s(t)$ or $\Omega_e \subseteq \Omega_L(t)$, respectively.
Also, the load vector \( F \) has dimension \( N_{\text{int}} \times 1 \). For each node \( A \) along \( \partial \Omega_0 \), we have that

\[
F^{A; \eta_{\text{int}}-1+\gamma} = \sum_{e=1}^{E_n} \int_{\partial \Omega_0} \Phi^\eta \mathbf{q} \, d\Gamma_e
\]

(21a)

where \( E_n \) is the number of elements which have one of their boundary segments lying on \( \partial \Omega_0 \) and \( q \) denotes the boundary flux.

The force vector for the interface nodes along the boundary \( \partial \Omega_i(t) \) is also accounted for by

\[
F^{A; \eta_{\text{int}}-1+\gamma} = \sum_{e=1}^{E_i} \int_{\partial \Omega_i} \Phi^\eta \left( R_k \frac{\partial \theta_S}{\partial n} - \frac{\partial \theta_L}{\partial n} \right) \, d\Gamma_e
\]

(21b)

where \( E_i \) is the total number of segments on the freezing front. The quantity inside the bracket of the equation above represents the flux discontinuity along the solid/liquid interface. As it will be shown later, equation (21b) will allow the determination of the interface velocity \( \mathbf{V} \) along \( \partial \Omega_i(t) \) when equated to the energy associated with the latent heat of fusion.

One should note the extra terms that arrive in the present formulation with respect to those in a standard Galerkin formulation. Also, one should notice the similarities of the present least-squares formulation with the streamlined Petrov–Galerkin formulations.\(^{26-29}\) In the present analysis, we neglect heat source terms, and as such the load term of the present formulation is the same as that of standard Galerkin formulations.

**Freezing front velocity calculation**

The calculation of the solid/liquid interface velocity follows that of Zabaras and Ruan.\(^{12}\) Consider that the boundary \( \partial \Omega_i(t) \) is broken up into \( E_i(t) \) boundary segments. Let \( N_{\text{int}} \) be the total number of nodes along \( \partial \Omega_i(t) \) with \( N_{\text{int}} \) the number of nodes in the interface segment \( e \). The interface velocity is now described over each segment with one-dimensional shape functions \( \Psi^\alpha \) as

\[
V_i = V_i^\alpha \Psi^\alpha \quad i = 1, 2, \quad \alpha = 1, \ldots, N_{\text{int}}^e
\]

(22)

The following weak form of the Stefan condition is introduced at time \( t_{\eta_{\text{int}}-1+\gamma} \):

\[
\sum_{e=1}^{E_i} \int_{\partial \Omega_i} \Psi^\alpha \left( R_k \frac{\partial \theta_S}{\partial n} - \frac{\partial \theta_L}{\partial n} \right) \, d\Gamma_e = \sum_{e=1}^{E_i} \int_{\partial \Omega_i} \Psi^\alpha \left( R_k \frac{\partial \theta_S}{\partial n} - \frac{\partial \theta_L}{\partial n} \right) \, d\Gamma_e
\]

(23)

By substituting equation (22) into equation (23) above, we have

\[
\sum_{e=1}^{E_i} \int_{\partial \Omega_i} \Psi^\alpha \Psi^\beta \left( R_k \frac{\partial \theta_S}{\partial n} - \frac{\partial \theta_L}{\partial n} \right) \, d\Gamma_e \mathbf{V}_i^\beta = \sum_{e=1}^{E_i} \int_{\partial \Omega_i} \Psi^\alpha \left( R_k \frac{\partial \theta_S}{\partial n} - \frac{\partial \theta_L}{\partial n} \right) \, d\Gamma_e
\]

(24)

where \( N_i^e \) is the \( i \)-th component of the unit normal vector to the \( e \)-th boundary segment along \( \partial \Omega_i(t) \).\(^{12}\) The right-hand side of equation (21b) is identical to that of equation (24). For every node \( A \) on \( \partial \Omega_i(t) \), we can write that

\[
\sum_{e=1}^{E_i} \int_{\partial \Omega_i} \Psi^\alpha \Psi^\beta \left( R_k \frac{\partial \theta_S}{\partial n} - \frac{\partial \theta_L}{\partial n} \right) \, d\Gamma_e \mathbf{V}_i^\beta = F^A
\]

(25)

where \( F^A \) is directly known from equation (19) once the temperature field has been calculated. Note that the melting temperature is applied as a boundary condition on \( \partial \Omega_i(t) \) and that \( F^A \) is obtained from the calculated temperature field in a way that is energy preserving.

To calculate the Cartesian components of the interface velocity, the nodal tangential velocities must be specified. In this work, the interface nodes are rearranged every few time steps so that
a well posed finite element mesh is preserved. After this operation is performed, the interface nodes are assumed to move in a direction normal to the interface.

**Incompressibility condition**

Here we use the consistent penalty method\textsuperscript{30} where the dynamic pressure term is eliminated from the momentum equations. The following weak form of equation (3) is used:

\[
\sum_{c=1}^{E} \int_{\Omega_e} \tilde{\Phi}^a p \, d\Omega_e = - \sum_{c=1}^{E} \int_{\Omega_e} \tilde{\Phi}^a \lambda (\nabla \cdot \mathbf{u}) \, d\Omega_e \tag{26}
\]

where the assembly is over the \(E\) elements in the liquid phase. Using the interpolation of the velocity field and assuming that there is no coupling between the pressure degrees of freedom between elements, we finally arrive at the following equation:

\[
p^\theta = - \lambda [\Pi_e^{-1}]^{\beta \mu} \int_{\Omega_e} \tilde{\Phi}^\mu \frac{\partial \Phi^\zeta}{\partial x_i} \, d\Omega_e \ u_i^\zeta \tag{27}
\]

where \(\alpha, \beta, \mu = 1, 2, \ldots, N^\text{red}\) (with \(N^\text{red}\) equal to the reduced number of pressure degrees of freedom per element \((N^\text{red} < N^\text{ele})\)), \(\zeta = 1, 2, \ldots, N^\text{ele}\) and

\[
\Pi_e^\theta = \int_{\Omega_e} \tilde{\Phi}^a \tilde{\Phi}^a \, d\Omega_e \tag{28}
\]

**The weak form of the momentum equations**

Let us denote with \(u_{j,n}\) the unknown \(j\)th velocity component \((j = 1, 2)\) at time \(t_n, n = 1, 2, \ldots\) and let us assume that \(u_{j,n-1}\) is known. In order to calculate \(u_{j,n}\) in a way similar to that presented for the energy equation, we introduce the residual \(R_j(u_{1;n}, u_{2;n})\) of equation (13) as

\[
R_j(u_{1:n}, u_{2:n}) = \frac{u_{j,n} - u_{j,n-1}}{\Delta t} + \frac{\partial u_j}{\partial x_m} \frac{\partial \Phi^a}{\partial x_m} \frac{\partial \Phi^a}{\partial x_m} \frac{\partial \Phi^a}{\partial x_m} + \frac{\partial p}{\partial x_j} \frac{\partial \Phi^a}{\partial x_j} \frac{\partial \Phi^a}{\partial x_j} - (\nabla \cdot [2 \text{ Pr} \text{ sym}(\nabla u_{n-1})])_{j,n-1} + \text{ Pr Re} \theta_{n-1,1} f_{j,n-1} \tag{29}
\]

The following least-squares optimization scheme is introduced:

\[
\sum_{c=1}^{E} \int_{\Omega_e} \frac{\partial R_j(u_{1:n}, u_{2:n})}{\partial u_{i,n}} \, d\Omega_e = 0 \quad \text{for} \quad \alpha = 1, 2, \ldots, N^\text{ele}, \quad i = 1, 2 \tag{30}
\]

The above equation can finally be written as

\[
\sum_{c=1}^{E} \int_{\Omega_e} \left[ \tilde{\Phi}^a \delta_{ij} + \gamma \Delta t \delta_{ij} \tilde{u}_{n-1,1} + \nabla \Phi^a \right] R_j(u_{1:n}, u_{2:n}) \, d\Omega_e \quad \text{for} \quad i = 1, 2 \tag{31}
\]

where the term \(\tilde{u}_{n-1,1}\) is kept constant in the minimization process (iteration will be performed on this term) and as before the additional contribution of the diffusive terms is neglected. With an integration by parts of the lower-order diffusive term in equation (31), neglecting the higher-order diffusive term, and using the constitutive equation (2) and the pressure equation (27), the following system of algebraic equations can finally be derived for the vector \(\{u_n\}\)
\[\{u_n\} = \{u_1, u_2, u_3, \ldots, u_n\}^T, \text{ with } n = N^{\text{liq}} \text{ (the number of nodes in the liquid phase)}:\]

\[\frac{\mathcal{M}_{n-1+\gamma}}{\Delta t} + \gamma (\mathcal{C}_{n-1+\gamma} + \mathcal{K}_{n-1+\gamma} + \mathcal{P}_{n-1+\gamma}) \{u_n\} + \left[\mathcal{D}_{n-1+\gamma}\right] \{\theta_{n-1+\gamma}\} = \{\mathcal{F}_{n-1+\gamma}\} + \left[\frac{\mathcal{M}_{n-1+\gamma}}{\Delta t} - (1 - \gamma)(\mathcal{C}_{n-1+\gamma} + \mathcal{K}_{n-1+\gamma} + \mathcal{P}_{n-1+\gamma})\right] \{u_{n-1}\}\]

(32)

where

\[\left[\mathcal{M}_{n-1+\gamma}\right] = \sum_{e=1}^{E_e} \left[\mathcal{M}_{e}^{n-1+\gamma}\right], \quad \left[\mathcal{C}_{n-1+\gamma}\right] = \sum_{e=1}^{E_e} \left[\mathcal{C}_{e}^{n-1+\gamma}\right], \quad \left[\mathcal{K}_{n-1+\gamma}\right] = \sum_{e=1}^{E_e} \left[\mathcal{K}_{e}^{n-1+\gamma}\right]\]

\[\left[\mathcal{P}_{n-1+\gamma}\right] = \sum_{e=1}^{E_e} \left[\mathcal{P}_{e}^{n-1+\gamma}\right], \quad \left[\mathcal{D}_{n-1+\gamma}\right] = \sum_{e=1}^{E_e} \left[\mathcal{D}_{e}^{n-1+\gamma}\right]\]

All matrices above expect \[\left[\mathcal{D}\right]\] have dimensions \(2N^{\text{liq}} \times 2N^{\text{liq}}\) and their components \((\alpha, \beta, \xi, = 1, \ldots, N^{\text{ele}}, i, j, m = 1, 2)\) are defined as:

\[\mathcal{M}_{e}^{i\alpha j\beta \cdot n-1+\gamma} = \int_{\Omega_e} \Phi^\alpha \delta_{ij} \Phi^\beta \ d\Omega_e + \int_{\Omega_e} \gamma \Delta t \delta_{ij} \bar{u}_{n-1+\gamma} \cdot \nabla \Phi^\alpha \Phi^\beta \ d\Omega_e\]  

(33a)

\[\mathcal{C}_{e}^{i\alpha j\beta \cdot n-1+\gamma} = \int_{\Omega_e} \bar{u}_{n-1+\gamma} \cdot \nabla \Phi^\beta \Phi^\alpha \delta_{ij} \ d\Omega_e + \int_{\Omega_e} \gamma \Delta t \delta_{ij} \bar{u}_{n-1+\gamma} \cdot \nabla \Phi^\alpha \bar{u}_{n-1+\gamma} \cdot \nabla \Phi^\beta \ d\Omega_e\]  

(33b)

\[\mathcal{K}_{e}^{i\alpha j\beta \cdot n-1+\gamma} = \int_{\Omega_e} Pr \delta_{ij} \nabla \Phi^\alpha \cdot \nabla \Phi^\beta \ d\Omega_e + \int_{\Omega_e} \frac{Pr}{\partial x_j} \frac{\partial \Phi^\alpha}{\partial x_i} \ d\Omega_e\]  

(33c)

and with \(\omega, \nu = 1, \ldots, N^{\text{red}},\)

\[\mathcal{P}_{e}^{i\alpha j\beta \cdot n-1+\gamma} = \lambda [\Pi_{e}^{-1}]^{\omega\nu} \int_{\Omega_e} \frac{\partial \Phi^\alpha}{\partial x_i} \Phi^\omega \ d\Omega_e \int_{\Omega_e} \Phi^\nu \frac{\partial \Phi^\beta}{\partial x_j} \ d\Omega_e\]  

(33d)

The matrix \([\mathcal{D}]\) has dimension \(2N^{\text{liq}} \times 2N^{\text{liq}}\) and is defined by

\[\mathcal{D}_{e}^{i\alpha j\beta \cdot n-1+\gamma} = \int_{\Omega_e} Pr Ra f_i \Phi^\alpha \Phi^\beta \ d\Omega_e + \int_{\Omega_e} \gamma \Delta t f_i Pr Ra \bar{u}_{n-1+\gamma} \cdot \nabla \Phi^\alpha \Phi^\beta \ d\Omega_e \quad \text{for } i = 1, 2\]  

(33e)

Finally, the load vector from boundary terms only is given as

\[\mathcal{F}_{e}^{i\alpha \cdot n-1+\gamma} = \sum_{e=1}^{E_e} \int_{\partial \Omega_e} \Phi^\alpha (\tau_{ij}(\bar{u}_0)) |_{n-1+\gamma} \ d\Gamma_e\]  

(33f)

Boundary conditions must be prescribed for equations (19) and (32). No slip velocity boundary conditions are prescribed along \(\partial \Omega_L(t)\) and \(\partial \Omega_i(t)\) and the melting temperature condition along \(\partial \Omega_i(t)\). Both heat flux and mixed temperature/flux conditions can be applied by appropriately computing the load vector \(\mathcal{F}\) along \(\partial \Omega_0\). For a mixed boundary condition, the stiffness matrix has to be modified.
Mesh generation

Due to the motion of the solid/liquid interface, $\partial \Omega_1(t)$, a time varying number of elements is utilized to discretize the domains $\Omega_s$ and $\Omega_L$. To demonstrate the method, let us consider the solidification problem. The region $\Omega_2(t)$ is divided into two sub-regions. In one of the subregions, the nodes are always stationary and in the other one, the nodes lying on the solid/liquid interface are moving with respect to time. The moving region includes only the elements of the solid phase next to the interface $\partial \Omega_1(t)$. These elements are allowed to change their sizes according to the movement of the interface front. When the sizes of these elements in the deforming region become larger than a prescribed size, a new moving region is generated by splitting up the deforming region into two separate regions (Figure 2). Interpolation is performed to calculate the new nodal temperatures. The region that lies next to the interface becomes the new deforming region while the other region is kept fixed in time. The new elements adjacent to the interface will continue deforming over the next time steps until once again a necessity exists for the introduction of new elements.

As the solid region grows and adapts to the solid/liquid interface with the creation of new elements, the liquid region $\Omega_1(t)$ shrinks and its remeshing may be necessary. The new nodal locations are generated by using a transfinite mapping technique. Mesh generation in the liquid region occurs at preset time steps (usually every three time steps or less) or when the interface nodes become irregular. The nodes become irregular when either the interface nodes move forward and cross over the next row or column of liquid elements (where all nodes but those on $\partial \Omega_1(t)$ are stationary), or when neighbouring interface nodes cross over each other. Both of these cases generate a negative Jacobian in the elements or bordering elements where the irregular nodes reside. Normally only the nodes along the interface have a nodal velocity associated with them based on the Stefan condition. However, a motion of the liquid nodes is introduced every

![Figure 2. Mesh generation scheme in the solid region: (a) mesh at time $t_{n-1}$ before new elements were created; (b) mesh at time $t_{n-1}$ after new elements were created; (c) mesh at time $t_n$ with new interface location](image-url)
time the liquid region is re-mapped. From the interface position at the previous time step, the
mesh in $\Omega_L(t)$ is re-mapped to fit better to the new geometry. This remeshing is considered to be
part of a nodal motion during the forthcoming time step. This significantly facilitates the
interpolation necessary during remeshing. Nodal velocities in $\Omega_L(t)$ are calculated by taking the
difference in the nodal co-ordinate positions between the time steps, and dividing them by the
current time step. Interface velocities along $\partial\Omega_L(t)$ and nodal velocities in $\Omega_L(t)$ both contribute to
the matrices in equations (19) and (32).

In unidirectional solidification where the interface stretches from the top to the bottom,
elements are removed from the liquid phase when new elements are created in the solid phase.
This preserves an equal number of elements for the entire mesh for all times. This is important
since a high number of elements is used in the liquid region and reducing the number of elements
as the program progresses will reduce the computation time.

When the liquid elements are reduced, interpolation is performed only in the liquid region to
transfer nodal values of temperature, material velocity and mesh velocity to the new nodes. Near
the end of the process when 90 per cent of the material has solidified, a substantial number of
elements is removed from the liquid region. The number of elements left in the liquid region
remains fixed until complete solidification is achieved.

Algorithm

At time $t_{n-1}$ assume the mesh geometry, nodal temperatures, material velocities and the
interface velocity are known. Then the algorithm at time $t_n$ includes the following steps:

For each time step $t_n = t_{n-1} + \Delta t$, $n = 1, 2, \ldots, (t_0 = 0)$

A. Determine if the sizes of the elements at $t = t_{n-1}$ in the deforming region of the solid phase
are equal to or less than a prescribed value.

1. If yes, the interface nodes are considered to move with the velocity $\{V_{n-1}\}$ calculated at
time $t = t_{n-1}$ while the non-interface nodes in the solid phase remain stationary.
   Check if the elements in the liquid phase at $t_{n-1}$ are substantially distorted.
   a. If yes, use transfinite mapping to define a new mesh in the melt region at $t_{n-1}$.
      The new nodal locations are considered to be the locations of nodes at time $t_n$.
      This is assumed to be part of a mesh motion from $t_{n-1}$ to $t_n$ as discussed earlier.
   b. If no, the nodes in the liquid phase remain stationary and only nodes on $\partial\Omega_L(t)$
      are assumed to have a non-zero velocity.

2. If no, new elements are added to the solid region and old elements are removed from the
   liquid region based on an earlier discussion. The required new nodal values at time
   $t_{n-1}$ are calculated from the old nodal values via an interpolation process.

B. For each iteration $i = 1, 2, \ldots$, maximum number of iterations

1. Calculate all matrices in equation (19), apply boundary conditions and solve for the
temperature field at $t_n$.
2. Using the calculated temperatures, calculate all matrices in equation (32), then apply
   boundary conditions and solve for the material velocity field at $t_n$.
3. Check the relative material velocity error as

$$\text{Error}_m = \frac{\|u_n(t)\| - \|u_n(t-1)\|}{\|u_n(t-1)\|}$$

(34)
where \( \| \cdot \| \) is the Euclidean norm of a vector and \( u_{n(i)} \) denotes the calculated vector of the material velocities on \( \Omega_L(t) \) at \( t_n \) after the \( i \)th iteration.

1. If \( \text{Error}_m < \text{tolerance} \), stop iteration (go to C).
2. If \( \text{Error}_m > \text{tolerance} \), continue iteration (return to B).

(Notahe that during the iterations B, the freezing interface location is not updated. This means that energy conservation is possibly not preserved at this stage).

C. For each iteration \( i = 1, 2, \ldots \), maximum number of iterations

1. Calculate all matrices in equation (19), then apply boundary conditions and solve for the temperature field at \( t_n \).
2. Using the calculated temperatures, calculate new interface velocities \( \{ V_{n(i)} \} \) using equation (25).
3. Update the location of the interface nodal points using
   \[
   \{ x_{n(i)} \} = \{ x_{n-1} \} + \Delta t \{ V_{n-1} + y(t) \}
   \]
4. Check the relative front velocity error as
   \[
   \text{Error}_f = \frac{\| V_{n(i)} \| - \| V_{n(i-1)} \|}{\| V_{n(i-1)} \|}
   \] (35)
   where \( V_{n(i)} \) denotes the calculated vector of the normal nodal velocities on \( \partial \Omega(t) \) at \( t_n \) after the \( i \)th iteration.
5. If \( \text{Error}_f < \text{tolerance} \), stop iteration (go to D).
6. If \( \text{Error}_f > \text{tolerance} \), continue iteration (return to C).

D. With the converged temperature field and interface location, solve iteratively equations (32) for the velocity field \( u_n \).

1. Check if both the freezing front velocity and the material velocity are acceptable (criteria of equations (34) and (35)).
2. If yes, go to E.
3. If no, return to step B.

E. Adjust time step
   1. If number of front iterations at \( t_n \) is less than number of front iterations at \( t_{n-1} \) and the number of front iterations at \( t_n \) is less than 5 then increase \( \Delta t \).
2. If number of front iterations at \( t_n \) is greater than number of front iterations at \( t_{n-1} \) and the number of front iterations at \( t_n \) is greater than 5 then reduce \( \Delta t \).

Continue time stepping unless time limit is reached.

To start the algorithm, a small finite solid region is assumed at time zero. Also, a special procedure is performed near the end of the solidification process, that allows \( \Omega_0 \) to completely solidify for the unidirectional case. First, when the node that coincides with the top or bottom of the interface boundary \( \partial \Omega_L(t) \) almost touches the corner of the mold, then that node is fixed as if it is a node in the solid region \( \Omega_S(t) \). The melting temperature boundary condition at the node that was just fixed is no longer applied (in essence this node is not anymore treated as the interface node). Thus the interface is reduced in size as it travels past the corner of the mold in the case of unidirectional solidification. After more time has elapsed, the next node that comes into close
contact with the wall (just above or below the node that was fixed) is also fixed and the prescribed melting temperature is not applied. This continues until solidification is approximately 99.5 per cent complete and the program halts. Although this method of reducing the front interface introduces some error, it occurs after most of the solidification process has been completed and thus this error is relatively small.

It is clear from the above discussion, that the present mesh generation/motion algorithm cannot account for multiple freezing fronts where new interfaces appear and disappear as well as for geometrically complicated casting/melting processes.

NUMERICAL RESULTS

In the following examples, bilinear shape functions were selected for temperature and velocity calculations and piece wise-constant shape functions for pressure calculations. A penalty number of $10^8$ was used for all cases reported. The first example is concerned with the solidification of pure aluminum in a square enclosure, while the second example is the melting of pure gallium in a rectangular enclosure.

Solidification of pure aluminum in a square region

Here, a square enclosure with aspect ratio of 1:0 is used. A mixed temperature/flux boundary condition was applied to one wall and all other walls were insulated (Figure 3). The square enclosure is initially occupied by liquid aluminum whose properties are given in Table I. The ambient temperature was taken as $\theta_\infty = -3.175$, while the Biot number is selected as $Bi = 3.3$. The dimensionless variables are given in Table II. The melt is initially superheated by an amount of $\Delta T = 200^\circ C$. The initial finite element mesh consists of 19 elements in the horizontal direction and 18 elements in the vertical (342 elements total), while the integration parameter was selected as $\gamma = 1$.

The first case analysed, corresponds to a Rayleigh number of $Ra = 10^5$. For this case, the dimensionless velocity and isotherms at different dimensionless times are shown in Figures 4(a)–4(d) and 5(a)–5(d), respectively. In the velocity field plots, the symbol $|u|_{ave}$ denotes the average magnitude of the velocity field, while $|u|_{max}$ is the maximum magnitude of the nodal
Table I. Thermal properties of pure aluminum

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat conductivity in solid</td>
<td>$K_S$</td>
<td>0.0548</td>
</tr>
<tr>
<td>Heat conductivity in liquid</td>
<td>$K_L$</td>
<td>0.0548</td>
</tr>
<tr>
<td>Specific heat in solid</td>
<td>$c_S$</td>
<td>2.526</td>
</tr>
<tr>
<td>Specific heat in liquid</td>
<td>$c_L$</td>
<td>2.526</td>
</tr>
<tr>
<td>Latent heat</td>
<td>$L_H$</td>
<td>95.0</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho$</td>
<td>2650</td>
</tr>
<tr>
<td>Kinematic viscosity</td>
<td>$\nu$</td>
<td>$1.22 \times 10^{-6}$</td>
</tr>
<tr>
<td>Thermal expansion coefficient</td>
<td>$\beta$</td>
<td>$3.84 \times 10^{-5}$</td>
</tr>
<tr>
<td>Melting temperature</td>
<td>$T_m$</td>
<td>660</td>
</tr>
<tr>
<td>Reference temperature</td>
<td>$T_0$</td>
<td>860</td>
</tr>
</tbody>
</table>

Figure 4. Dimensionless velocity fields for the solidification example with $Ra = 10^5$: (a) $t = 0.05$, $|u|_{ave} = 5.1$, $|u|_{max} = 24.1$; (b) $t = 0.15$, $|u|_{ave} = 6.7$, $|u|_{max} = 26.1$; (c) $t = 0.35$, $|u|_{ave} = 2.4$, $|u|_{max} = 15.5$; (d) $t = 0.60$, $|u|_{ave} = 0.1$, $|u|_{max} = 1.9$
velocity vectors. Note that the arrow scale for the velocity field in each of the cases of Figures 4(a)–4(d) is the same. Clearly the freezing interface curves due to natural convection. The solidification growth is faster near the bottom of the enclosure. The velocity field is shown to grow as the process proceeds in time reaching a peak before it eventually dies out. The results shown in Figures 4(a)–4(d) are very similar to the ones presented by Yoo and Rubinsky, who analysed the
problem under very similar conditions. However, they only reported results at the early stages of solidification. The predicted separation of flow shown in Figures 4(b) and 4(c) and the weaker but numerically stable secondary convection cells, on the upper right hot part of the melt and the lower right corner region, were not observed at lower $Ra$ numbers.

To investigate the effect of $Ra$ number on melt flow and the temperature field, the case of $Ra = 10^6$ is examined. All other properties are the same as in the case of $Ra = 10^7$. The initial finite element mesh consists of 21 elements in the horizontal direction and 20 elements in the vertical (420 elements total). The interface morphology, melt flow and temperature field, are strongly affected by the Rayleigh number. This is shown in Figures 6(a)–6(d) and 7(a)–7(d), where the velocity and temperature fields are shown for the case of $Ra = 10^6$. The scale for the velocity field in each of the cases Figures 6(a)–6(d) is the same, but different from the scale used in Figures 4(a)–4(d). The melt flow in Figures 6(a)–6(d) is much stronger and is developed differently than that of Figures 4(a)–4(d) while significant differences also appear in the temperature fields of the

![Figure 6. Dimensionless velocity fields for the solidification example with $Ra = 10^6$: (a) $t = 0.05$, $|u|_{ave} = 23.1$, $|u|_{max} = 105.1$; (b) $t = 0.15$, $|u|_{ave} = 9.9$, $|u|_{max} = 51.4$; (c) $t = 0.35$, $|u|_{ave} = 3.6$, $|u|_{max} = 22.0$; (d) $t = 0.60$, $|u|_{ave} = 0.2$, $|u|_{max} = 2.0$.](image-url)
two $Ra$ number cases. Several weak (but numerically stable) secondary flow cells are observed as in the case of $Ra = 10^5$. Due to the selected resolution for the velocity field, these secondary cells are barely recognizable in Figures 6(b)–6(c). Also note that the secondary flow cells appear much earlier in the case of $Ra = 10^6$ than in the case of $Ra = 10^5$. Figure 8 presents a comparison of the freezing front positions for the cases $Ra = 0$ (Stefan problem), $10^4$, $10^5$, $10^6$. The initial finite element mesh for the cases of $Ra = 0$ and $Ra = 10^4$ was the same as in the case of $Ra = 10^5$. The obtained results shown in Figure 8 are very similar with those of Reference 19.

Finally, Table III gives the dimensionless total solidification times for the four different $Ra$ number cases mentioned earlier. With respect to the total dimensionless solidification time for the case of no convection ($Ra = 0$), the total dimensionless solidification time increased for $Ra = 10^4$, but decreased for $Ra = 10^5$ and $Ra = 10^6$. The flow separation that occurs at high $Ra$ numbers affects the temperature distribution for later solidification times and effectively pulls the upper part of the solid/liquid interface forward. Thus the solidification time is reduced.
Figure 8. Comparison of freezing front locations at different dimensionless times for four \( Ra \) number cases

Table III. Total dimensionless solidification times

<table>
<thead>
<tr>
<th>Example</th>
<th>Total time</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Ra = 0.000 )E0</td>
<td>0.840</td>
</tr>
<tr>
<td>( Ra = 1.000 )E4</td>
<td>0.847</td>
</tr>
<tr>
<td>( Ra = 1.000 )E5</td>
<td>0.833</td>
</tr>
<tr>
<td>( Ra = 1.000 )E6</td>
<td>0.813</td>
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</table>

Table IV. Thermal properties of pure gallium

<table>
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<tr>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat conductivity in solid</td>
<td>( K_s )</td>
<td>32.0</td>
</tr>
<tr>
<td>Heat conductivity in liquid</td>
<td>( K_l )</td>
<td>32.0</td>
</tr>
<tr>
<td>Specific heat in solid</td>
<td>( c_s )</td>
<td>381.5</td>
</tr>
<tr>
<td>Specific heat in liquid</td>
<td>( c_l )</td>
<td>381.5</td>
</tr>
<tr>
<td>Latent heat</td>
<td>( L_H )</td>
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</tr>
<tr>
<td>Density</td>
<td>( \rho )</td>
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</tr>
<tr>
<td>Kinematic viscosity</td>
<td>( \nu )</td>
<td>( 1.81 \times 10^{-3} )</td>
</tr>
<tr>
<td>Thermal expansion coefficient</td>
<td>( \beta )</td>
<td>( 1.20 \times 10^{-4} )</td>
</tr>
<tr>
<td>Melting temperature</td>
<td>( T_m )</td>
<td>29.78</td>
</tr>
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</table>

Table V. Dimensionless variables for pure gallium

<table>
<thead>
<tr>
<th>Symbol</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Prandtl number</td>
<td>( Pr )</td>
</tr>
<tr>
<td>Rayleigh number</td>
<td>( Ra )</td>
</tr>
<tr>
<td>Stefan number</td>
<td>( Ste )</td>
</tr>
<tr>
<td>Heat conductivity ratio</td>
<td>( R_K )</td>
</tr>
<tr>
<td>Specific heat ratio</td>
<td>( R_C )</td>
</tr>
</tbody>
</table>
Figure 9. Melting of gallium in a rectangular enclosure

Figure 10. Dimensionless velocity fields for the melting of gallium example: (a) $t = 2.04$, $|u|_{ave} = 12.7$, $|u|_{max} = 44.5$;
(b) $t = 3.26$, $|u|_{ave} = 13.1$, $|u|_{max} = 44.5$; (c) $t = 4.89$, $|u|_{ave} = 13.8$, $|u|_{max} = 43.3$
Melting of gallium in a rectangular region

For a melting problem, buoyancy-induced natural convection plays a much stronger role on the shape of the solid/liquid interface. Gau and Viskanta\textsuperscript{34} have performed experiments for melting of pure metal gallium with buoyancy-induced flow and have measured the effect of convection on the solid/liquid interface motion. This problem was studied by Brent et al.\textsuperscript{35} using the enthalpy method with finite differences and a fixed grid and by Lacroix and Voller\textsuperscript{22} who used fixed-grid and transformed-grid techniques. The material properties for pure gallium are shown in Table IV.

The melting experiment is modeled in a vertical, two-dimensional rectangular enclosure of aspect ratio = 2 (height = 0.045 m, width = 0.09 m). Constant boundary temperature conditions are applied to the vertical walls where on the left wall $T = T_H = 38.6^\circ$C and on the right wall $T = T_m = 29.8^\circ$C (melting temperature). The top and bottom walls were insulated. The initial temperature condition was the melting temperature $T_m$. By setting the dimensional length to $L = 0.045$ m and the temperature variable $T_0 = T_H$, the dimensionless variables are calculated and given in Table V. The dimensionless boundary conditions and geometry for the melting example are shown in Figure 9.

The number of elements in the liquid region was held fixed. Transfinite mapping was performed in every step to allow elements to adjust naturally to the solid/liquid interface. The energy

Figure 11. Dimensionless temperature fields for the melting of gallium example: (a) $t = 2.04$; (b) $t = 3.26$; (c) $t = 4.89$
equation in the solid domain was not needed as the solid temperature remained constant at all times. The initial finite element mesh consisted of 2 elements in the horizontal direction and 18 elements in the vertical (36 elements total). The integration parameter was selected as \( \gamma = 0.75 \).

Figures 10(a)–10(c) and 11(a)–11(c) show the dimensionless velocity field and isotherms at three different dimensionless times, respectively. In Figure 12, the calculated front location history is shown to compare well with the experimental results, and the transformed-grid technique of Lacroix and Voller. Finally, Figure 13 shows the calculated melting front locations at different dimensionless times using three different integration parameters (\( \gamma = 0.5, 0.75, 1 \)). It is not easy to compare the accuracy of these three cases since the time step within each case was continuously adjusted by the algorithm.

Figure 12. Comparison of melting front locations at different dimensionless times

Figure 13. Calculated melting front location using different integration parameters
CONCLUSIONS

A least-squares front-tracking finite element model for phase-change problems with natural convection was developed. The transient Navier–Stokes equations were coupled to the transient energy equations and the Stefan condition. Deforming finite elements were utilized for compatibility between the solid and liquid domains which preserved energy and allowed boundary conditions along the interface to be prescribed exactly. The bulk fluid motion was generated using the Boussinesq approximation. The consistent penalty method was developed for incompressibility. The least-squares formulation was able to account for convection dominated solidification and melting processes without any deleterious numerical effects. A generalized mid-point type of temporal integration rule was used and the results were shown to be stable and accurate for 0.5 ≤ γ ≤ 1.

In addition to the main flow cell observed in the solidification example, at high Ra numbers, other secondary stable but weaker cells were observed as well. The unstable eddies at the early time stage of the melting example reported in Reference 36 were also observed in our investigations when the regular Galerkin formulation was implemented. These unstable structures obtained using the regular Galerkin formulation, eventually resulted in numerical oscillation of the velocity field. This can be attributed to either a coarse mesh or more possibly to false diffusion in a convection dominated environment. No such unstable cells were observed while using the present least-squares formulation. The 'streamline upwinding' that was naturally introduced in the least-squares formulation did not suppress all secondary eddies even for the rather coarse mesh cases presented in this paper. In the melting example, the secondary cell that was observed at the lower right corner of the liquid region was significantly weaker than the main convection cell, and as such our results were found to be much closer to those of Voller and colleagues.22

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REFERENCES


