Boundary integral equation solution of steady natural convection in solid-liquid systems

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Abstract

This paper describes a primitive variable boundary integral equation solution of the free boundary problem arising in the steady natural convection of the incompressible Newtonian solid-liquid phase change material. Solution of the coupled mass, momentum, and energy equations in two-dimensions is structured by the fundamental solution of the Laplace equation, straight line geometry and discontinuous linear field boundary elements. The involved domain integrals are treated through the dual reciprocity transformation based on the scaled augmented thin plate splines.

1 Introduction and Motivation

Various aspects of science and technology are nowadays related to modelling of the solid-liquid phase change systems. The boundary integral methods have been in the past applied [1] only to the solution of specific aspects of melting and solidification. One of the primary goals of our current research is the boundary integral solution of the general one-phase mixture model [2] of heat, mass, momentum, and species transfer in such systems. The heat transfer part of the problem has been worked out in [3, 4] by the Dual Reciprocity Boundary Element Method (DRBEM) [5]. This development already found industrial application [6] within modelling of the direct-chill casting of alluminium alloy billets. The boundary integral formulation of the problem of mass and momentum transport in solid-liquid phase change systems has been represented in [7]. The numerical implementation of the liquid phase part of the problem has been elaborated in [8]. This paper
shows testing of the formulation for steady natural convection in single-phase fluid and phase change material.

2 Governing Equations

This paper deals with incompressible Newtonian solid-liquid phase change material confined in the domain $\Omega$ with the boundary $\Gamma$. The mass, momentum, and energy conservation for the defined system is

$$\nabla \cdot \mathbf{v} = 0$$ (1)

$$\rho \nabla \cdot (\mathbf{v} \mathbf{v}) = -\nabla P + \mu \nabla^2 \mathbf{v} + \mathbf{f}$$ (2)

$$\rho c_p \nabla \cdot (\mathbf{v} T) = k \nabla^2 T$$ (3)

with $\mathbf{v}$ standing for velocity, $P$ for pressure, and $T$ for mixture temperature. The involved material properties are constant density $\rho$, viscosity $\mu$, specific heat at constant pressure $c_p$, and thermal conductivity $k$. The variation of the density with temperature is included in the body force term only by using the Boussinesq approximation

$$\mathbf{f} = \rho \mathbf{a} \left( 1 - \beta (T - T_{\text{ref}}) \right) - c_p \left( 1 - f_L(T) \right) \mathbf{v}$$ (4)

with $\mathbf{a}$ standing for the acceleration vector, $\beta$ for the volumetric thermal expansion coefficient, and $T_{\text{ref}}$ for the reference temperature. The second term in the body force is modelling the phase change, simply constituted through the phase change coefficient $c_p$ and the temperature dependent liquid fraction $f_L$ which is assumed to vary as

$$f_L(T) = \begin{cases} 0 & T < T_S \\ (T - T_S)/(T_L - T_S) & T_S \leq T \leq T_L \\ 1 & T > T_L \end{cases}$$ (5)

where $T_S$ stands for the solidus, and $T_L$ for the liquidus temperature.

The solution of the equations (1,2,3) is constructed by defining the Dirichlet and Neumann velocity and temperature boundary conditions on the not necessarily connected parts of the boundary $\Gamma^D_v$, $\Gamma^N_v$, $\Gamma^D_T$, $\Gamma^N_T$

$$\mathbf{v} = \mathbf{v}_D; \quad \mathbf{p} \in \Gamma^D_v$$ (6)

$$\frac{\partial \mathbf{v}}{\partial \mathbf{n}_\Gamma} = \mathbf{v}_N; \quad \mathbf{p} \in \Gamma^N_v$$ (7)

$$T = T_D; \quad \mathbf{p} \in \Gamma^D_T$$ (8)

$$\frac{\partial T}{\partial \mathbf{n}_\Gamma} = T_N; \quad \mathbf{p} \in \Gamma^N_T$$ (9)

where $\mathbf{p}$ stands for the position vector, $\mathbf{n}_\Gamma$ for the normal on the boundary $\Gamma$, and $\mathbf{v}_D$, $\mathbf{v}_N$, $T_D$, and $T_N$ denote known functions. The solution of the posed natural convection problem represents the velocity, pressure, and temperature distribution over the domain $\Omega$ and the boundary $\Gamma$. 

3 Solution Procedure

The construction of the solution procedure is represented in two steps. The first step involves conversion of the partial differential equations into integral equations as well basic elements of the iterative procedure. The second step focuses on the discretization, setup and solution of the algebraic systems of equations. The momentum equation is coupled with the energy equation through the body force. The energy equation is coupled with the momentum equation through the velocity field. Consequently, the solution inherently involves iterations. The solution steps are explained in a continuous setting, where no reference need to be made regarding the discretization that is explained afterwards.

3.1 Integral Equations

Let us assume the velocity, pressure and temperature fields are all known at iteration level \( m \). The discussion of iteration cycle that follows explains how the velocity, pressure and temperature fields are calculated at the next iteration level \( m + 1 \). The solution of the momentum equation at the iteration level \( m + 1 \) is obtained in the following way: The Pressure Poisson Equation (PPE) is constructed by taking the divergence of the momentum (2) conservation

\[
\nabla^2 p^{m+1} = \nabla \cdot S_P^m
\]

with \( S_P^m \) standing for

\[ S_P^m = -\varepsilon \nabla \cdot (\nu v^m) + \mu \nabla^2 v^m + \varepsilon a (1 - \beta (T^m - T_{ref}))-c_P (1 - f_E^m) v^m \]

The Neumann pressure boundary conditions can be defined on the whole boundary \( \Gamma \) by taking the scalar product of the momentum equation with the normal on the boundary. This gives

\[
\frac{\partial p^{m+1}}{\partial n} = S_P^m \cdot n; \; p \in \Gamma
\]

The PPE with the boundary conditions (12) is solved by weighting the equation (10) with the fundamental solution of the Laplace equation \( T^*(p; s) \) (where parameter \( s \) stands for the source point position) over the domain \( \Omega \). This gives the following integral equation after application of the Green’s second identity for scalars

\[
\int_\Gamma \frac{\partial p^{m+1}}{\partial n} T^* d\Gamma - \int_\Gamma P^{m+1} \frac{\partial T^*}{\partial n} d\Gamma - c_s^* S_P^{m+1} = \int_\Omega \nabla \cdot S_P^m T^* d\Omega
\]

Subscript \( s \) denotes evaluation of a quantity at the source point \( s \). \( c_s^* \) stands for the fundamental solution related coefficient. Numerical implementation is in the present paper limited to two-dimensional Cartesian system, e.g.

\[
T^* = \frac{1}{2\pi} \log \frac{r_0}{r}
\]
where $r_0$ represents the reference radius, and $r$ equals to

$$r^2 = \mathbf{r} \cdot \mathbf{r}; \quad r = r_x \mathbf{i}_x + r_y \mathbf{i}_y; \quad r_x = p_x - s_x, \quad r_y = p_y - s_y$$

$p_x, p_y$ denote Cartesian coordinates (base vectors $\mathbf{i}_x, \mathbf{i}_y$) of point $p$, and $s_x, s_y$ Cartesian coordinates of fundamental solution source point $s$ respectively.

Equation (13) is first used for determining the pressure distribution on the boundary $\Gamma$ and subsequently explicitly in the domain $\Omega$. The pressure gradients on the boundary and in the domain can be explicitly calculated from the pressure gradient Poisson equation

$$\int_{\Gamma} \frac{\partial P}{\partial n\Gamma} T^* d\Gamma - \int_{\Gamma} P^{m+1} \frac{\partial T^*}{\partial n\Gamma} d\Gamma + \nabla (c_s^* P_s^{m+1}) = \int_{\Omega} \nabla \cdot S_p^m \nabla T^* d\Omega$$

obtained by taking the gradient of the PPE acting on the fundamental solution source point. After calculating the pressure gradient field the velocity field at iteration level $m+1$ can be calculated from the momentum equation. The momentum equation with the boundary conditions (6,7) is solved by weighting the equation (2) with the fundamental solution of the Laplace equation over the domain $\Omega$. This gives the following integral equation after application of the Green’s second identity for vectors

$$\int_{\Gamma} \frac{\partial \hat{\mathbf{v}}}{\partial n\Gamma} \cdot T^* d\Gamma - \int_{\Gamma} \hat{\mathbf{v}}^{m+1} \frac{\partial T^*}{\partial n\Gamma} d\Gamma - c_s^* \hat{\mathbf{v}}_s^{m+1} = \int_{\Omega} S_v^m \nabla T^* d\Omega$$

with $S_v^m$ standing for

$$S_v^m = \frac{1}{\mu} \left[ \rho \nabla \cdot (\hat{\mathbf{v}}^{m+1}) + \nabla P^{m+1} - \rho a (1 - \beta (T^{m} - T_{ref})) + c_p (1 - f_L^m) \hat{\mathbf{v}}^{m+1} \right]$$

The ”hat” on the velocity denotes that the velocity field does not correspond to the mass conservation in general. Equation (17) is used for simultaneous determination of the velocity gradients on the boundary $\Gamma$ and velocity in the domain $\Omega$. The velocity gradients on the boundary and in the domain can be explicitly calculated from the velocity gradient Poisson equation

$$\int_{\Gamma} \frac{\partial \hat{\mathbf{v}}}{\partial n\Gamma} \cdot T^* d\Gamma - \int_{\Gamma} \hat{\mathbf{v}}^{m+1} \frac{\partial T^*}{\partial n\Gamma} d\Gamma + \nabla (c_s^* \hat{\mathbf{v}}_s^{m+1}) = \int_{\Omega} S_v^m \nabla T^* d\Omega$$

The second derivatives $\frac{\partial^2 \hat{\mathbf{v}}^{m+1}}{\partial x^2}$ and $\frac{\partial^2 \hat{\mathbf{v}}^{m+1}}{\partial y^2}$ on the boundary that are needed in evaluation of the boundary condition (12) can be explicitly calculated from the integral representation

$$\int_{\Gamma} \frac{\partial \hat{\mathbf{v}}}{\partial n\Gamma} \frac{\partial}{\partial p_\xi} \nabla T^* d\Gamma - \int_{\Gamma} \hat{\mathbf{v}}^{m+1} \frac{\partial}{\partial p_\xi} \nabla T^* d\Gamma + \frac{\partial}{\partial p_\xi} \nabla (c_s^* \hat{\mathbf{v}}_s^{m+1}) = \int_{\Omega} S_v^m \frac{\partial}{\partial p_\xi} \nabla T^* d\Omega$$

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The incompressibility is enforced through the pressure $\tilde{P}^{m+1}$ and velocity $\tilde{v}^{m+1}$ correction which ensures

$$\nabla \cdot \mathbf{v}^{m+1} = \nabla \cdot (\tilde{v}^{m+1} + \tilde{v}^{m+1}) = 0$$  \hspace{1cm} (21)

Consider that the velocity correction $\tilde{v}^{m+1}$ occurs exclusively due to action of the pressure correction $\tilde{P}^{m+1}$

$$\frac{\theta}{\Delta t} \tilde{v}^{m+1} = -\nabla \tilde{P}^{m+1}$$  \hspace{1cm} (22)

with $\Delta t$ standing for heuristic velocity-pressure correction relaxation factor. The pressure correction can thus be calculated from the velocity field $\tilde{v}^{m+1}$ through the pressure correction Poisson equation

$$\nabla^2 \tilde{P}^{m+1} = \frac{\theta}{\Delta t} \nabla \cdot \mathbf{v}^{m+1}$$  \hspace{1cm} (23)

deduced from equations (21) and (22). The boundary-domain integral equivalent for solving the pressure correction Poisson equation is

$$\int_{\Gamma} \frac{\partial \tilde{P}^{m+1}}{\partial n_\Gamma} T^* d\Gamma - \int_{\Gamma} \tilde{P}^{m+1} \frac{\partial T^*}{\partial n_\Gamma} d\Gamma - c^* \tilde{P}_s^{m+1} = \int_{\Omega} \frac{\theta}{\Delta t} \nabla \cdot \mathbf{v}^{m+1} T^* d\Omega$$  \hspace{1cm} (24)

with the pressure correction Poisson equation Neumann boundary conditions

$$\frac{\partial \tilde{P}^{m+1}}{\partial n_\Gamma} = 0; \quad p \in \Gamma$$  \hspace{1cm} (25)

The pressure correction gradient $\nabla \tilde{P}^{m+1}$ on the boundary and in the domain can be explicitly calculated from the integral representation

$$\int_{\Gamma} \frac{\partial \tilde{P}^{m+1}}{\partial n_\Gamma} \nabla T^* d\Gamma - \int_{\Gamma} \tilde{P}^{m+1} \nabla \frac{\partial T^*}{\partial n_\Gamma} d\Gamma + \nabla (c^* \tilde{P}_s^{m+1}) = \int_{\Omega} \frac{\theta}{\Delta t} \nabla \cdot \tilde{v} \nabla T^* d\Omega$$  \hspace{1cm} (26)

The pressure and pressure gradient fields are updated as

$$P^{m+1} = P^{m+1} + \tilde{P}^{m+1}$$

$$\nabla P^{m+1} = \nabla P^{m+1} + \nabla \tilde{P}^{m+1}$$  \hspace{1cm} (27)

The velocity field is updated through the pressure gradient corrections

$$\mathbf{v}^{m+1} = \mathbf{v}^{m+1} - \frac{\Delta t}{\theta} \nabla \tilde{P}^{m+1}$$  \hspace{1cm} (28)

The iteration cycle is completed by calculating the temperature field at iteration level $m + 1$ (and with this also $f^{m+1}$). This is accomplished by
weighting the energy conservation equation by the fundamental solution of the Laplace equation and by using the Green’s second identity for scalars

\[ \int_{\Gamma} \frac{\partial T}{\partial n} m+1 T^* d\Gamma - \int_{\Gamma} T^m+1 \frac{\partial T^*}{\partial n} d\Gamma - c_s T^m+1 = \]

\[ = \int_{\Omega} \frac{1}{\alpha} \nabla \cdot \left( \nabla m+1 T^m+1 \right) T^* d\Omega \] (29)

with \( \alpha = k/(\rho c_p) \) denoting thermal diffusivity. Equation (29), together with the thermal boundary conditions (8,9), is used to simultaneously solve the unknown temperature distribution in the Neumann part of the boundary, the unknown temperature derivative in the normal boundary direction in the Dirichlet part of the boundary and unknown temperatures in the domain. The iteration cycle is completed with calculation of the updated temperature dependent Boussinesq and phase change terms

\[ f^{m+1} = \rho a \left( 1 - \beta \left( T^{m+1} - T_{\text{ref}} \right) \right) - c_p \left( 1 - f_L(T^{m+1}) \right) v^{m+1} \] (30)

The iterations are stopped when conditions

\[ \frac{||v^{m+1}|| - |v^m|}{|v^m|} < v_\epsilon \quad \frac{||T^{m+1}|| - |T^m|}{|T^m|} < T_\epsilon \] (31)

are satisfied with \( v_\epsilon \) and \( T_\epsilon \) representing the velocity and temperature convergence criteria. In case iteration conditions (31) are not satisfied, a new iteration cycle starts with the relaxed value of the body force with \( c_{\text{rel}} \) representing the heuristic relaxation factor

\[ f^{m+1} = f^m + c_{\text{rel}} \left( f^{m+1} - f^m \right) \] (32)

### 3.2 Numerical Implementation

The velocity, pressure, and temperature fields are all calculated in the same gridpoints \( p_n; n = 1, 2, \ldots, N; N = N_\Gamma + N_\Omega \). The first \( N_\Gamma \) gridpoints are distributed on the boundary and the last \( N_\Omega \) in the domain. Boundary geometry is approximated by \( N^\Gamma \) straight line segments, and spatial variation of the fields on each of the boundary segments is represented by the discontinuous linear interpolation functions i.e., \( N_\Gamma = 2 N^\Gamma \). The domain integrals in equations (13,16,17,19,20,24,26,29) are transformed by considering the approximation of the spatial variation of the field \( F \) over \( \Omega \) by the global interpolation functions \( \psi_n \) and their coefficients \( \zeta_n \)

\[ F(p) \approx \psi_n(p) \zeta_n; \quad n = 1, 2, \ldots, N + 3 \] (33)

The two-dimensional scaled augmented thin plate splines are used in this work

\[ \psi_n(p) = r_n^2 \log r_n; \quad n = 1, 2, \ldots, N \]

\[ \psi_{N+1}(p) = p_x - p_x^0 \quad \psi_{N+2}(p) = p_y - p_y^0 \quad \psi_{N+3}(p) = 1 \]
\[ r^2_n = (p - p_n) \cdot (p - p_n) \]  \hspace{1cm} (34)

The scaling constants \( p_x^0 \) and \( p_y^0 \) have been set to

\[ p_x^0 = \frac{1}{2} \left( p_{x_{\text{max}}} + p_{x_{\text{min}}} \right) \quad p_y^0 = \frac{1}{2} \left( p_{y_{\text{max}}} + p_{y_{\text{min}}} \right) \]  \hspace{1cm} (35)

where \( p_{x_{\text{max}}}, p_{y_{\text{max}}} \) represent the maximum and \( p_{x_{\text{min}}}, p_{y_{\text{min}}} \) the minimum coordinates \( p_x, p_y \) respectively of the domain \( \Omega \). The involved systems of linear equations that originate from solution of the integral equations are in present work solved by standard subroutines from [9]. The regular \( N \times N \) systems of linear equations that originate from integral equations (17,29) are solved by LU decomposition and backsubstitution by using subroutines LUDCMP and LUBKSB. The \( N_T \times N_T \) systems that originate from integral equations (16,26) are singular since the pressure and pressure corrections are known only up to an additive constant. This two systems are thus solved by Householder reduction to bidiagonal form and QR diagonalization with shifts by using subroutines SVDCMP and SVBKSB. The temperature and velocity tolerances have been set to \( 10^{-3} \, [\text{m/s}] \) and \( 10^{-3} \, [\text{K}] \). All involved boundary integrals are solved analytically [10]. Other discretization details of the involved boundary-domain integral equations can be found in [8].

### 4 Numerical Examples

Two numerical examples are shown in the present text. They are represented in the dimensional form because of the space constraints. Geometry is a square with dimension \( 1 \, [\text{m}] \). Upper and lower boundaries are insulated, the left boundary is subject to temperature \(-0.5 \, [\text{C}]\) and the right boundary is subject to temperature \(+0.5 \, [\text{C}]\). Phase change coefficient \( c_P \) is set to \( 0 \, [\text{kg/m}^{-3} \, \text{s}^{-1}] \) in case of the single-phase fluid and to \( 10^5 \, [\text{kg/m}^{-3} \, \text{s}^{-1}] \) in case of the phase change material. The solidus and the liquidus temperatures are \( T_S = -0.01 \, [\text{C}] \), \( T_S = +0.01 \, [\text{C}] \). All other material properties except \( \beta = 10^4 \, [1/\text{K}] \) are set to unit values. The square is discretized into 120 boundary elements and 841 domain nodes that give 1081 meshpoints. Heuristic parameters have been set to \( \Delta t = 1 \, [\text{s}] \) and \( c_{rel} = 0.1 \). Figures 1 and 2 show solution of the natural convection with the single-phase fluid and the phase change material, respectively. Solution in Figures 1 and 2 reach steady state after 85 and 61 iterations. A proper single-phase fluid numerical implementation is confirmed by matching with the classical [11] benchmark. A proper phase-change numerical implementation is confirmed by matching with the very recent results obtained by the finite volume method described in Appendix IX of [12]. A systematic comparative study of these two methods will appear elsewhere.

### 5 Conclusions

This preliminary study shows basic elements of the DRBEM based computational modelling of the natural convection in phase change materials as
Figure 1: Isotherms and velocity vectors of the natural convection in a square cavity. Example with the single-phase fluid. Maximum velocity is 19.6 [m/s].

required in numerous natural and technological systems. It probably represents the first attempt to solve a solid-liquid phase change problem including natural convection in the liquid phase by any boundary integral equation based discrete approximate method. The example represented in Figure 2 mimics (narrow phase change interval) the phase change of a pure substance, a problem that is usually difficult to solve with a fixed-grid technique. The developed method however demonstrates stability even for much coarser discretization and flow intensity as used in the present paper. This development is, due to the simple unstructured mesh and involved boundary integrations only, particularly advantageous in geometrically complicated systems and systems where one coordinate extends to infinity. However, realistic situations require upgrading of numerical implementation to ax-
Figure 2: Isotherms and velocity vectors of the natural convection in a square cavity. Example with the phase change material. Maximum velocity is $11.5 \text{m/s}$.

isymmetry [13] and to three dimensions as well use of the iterative methods for solution of the involved large systems of algebraic equations [14].

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