



Boundary integral formulation of general source-based method for convective-diffusive solid-liquid phase change problems

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Abstract

A new one-domain dual reciprocity boundary integral method technique for solving one-phase continuum formulation of the convective-diffusive energy equation as appears when treating energy transport in solid-liquid phase change systems is described. Laplace equation fundamental solution weighting, straight line geometry and constant field shape functions on the boundary, Crank-Nicolson time discretization and thin plate splines for transforming the domain integrals into a finite series of boundary integrals are employed. Iterations over the timestep are based on the Voller-Swaminathan scheme, upgraded to cope with the convective term. The technique could be applied to a wide range of solid-liquid phase change problems where finite volume or finite element solvers have been almost exclusively used in the past.

1. Introduction

Various aspects of science and technology are related to the prediction of transport phenomena in solid-liquid phase change systems. The discipline was established by Lamé, Clapeyron, Neumann and Stefan in the last century (Šarler [1]). Boundary integral methods have been extensively used in solving a wide range of melting and solidification problems (Šarler et al.[2]). Nowadays, the majority (Šarler [3]) of the solid-liquid phase change models for describing macroscopic transport phenomena rely on one-phase continuum formulation (Bennon et al.[4], Ni et al.[5]). However, the solution procedures for solving such problems have been almost exclusively confined to established finite volume or finite element techniques. The exception is presented in our previous works where the boundary integral formulation of

the coupled mass, momentum, energy and species transfer problem has been deduced (Šarler et al.[6]). The formulation of convective-diffusive problems by using weighting with the fundamental solution of Laplace and Fourier equations has been presented in (Šarler et al.[7]) and solved by the dual reciprocity method for diffusive (Šarler et al.[8]) and convective-diffusive (Šarler et al.[9]) constant density phase-change problems based on Kirchhoff variable formulation and heuristic global interpolation functions.

In this work the physics of the problem is made more general, allowing for variation of all material properties, the solution procedure is changed to the Kirchhoff variable-Liquid volume fraction formulation, and optimum thin plate spline global interpolation functions are used. The principal aim of this paper is to elaborate the new, relatively involved formulation of the problem, leaving the already performed extensive checking of the technique to be presented in one of our next papers.

2. Governing Equations

Consider a connected fixed domain Ω with boundary Γ occupied by a phase change material described with the temperature dependent density $\rho_{\mathcal{P}}$, specific heat at constant pressure $c_{\mathcal{P}\mathcal{P}}$ and the thermal conductivity $k_{\mathcal{P}}$ of the solid $\mathcal{P} = s$ and the liquid $\mathcal{P} = \mathcal{L}$ phase, and the specific latent heat of the solid-liquid phase change $h_{\mathcal{M}}$. The one-phase continuum formulation of the energy transport for the assumed system is

$$\begin{aligned} \frac{\partial}{\partial t}(f_S \rho_S h_S + f_L \rho_L h_L) + \nabla \cdot (f_S \rho_S h_S \mathbf{V}_S + f_L \rho_L h_L \mathbf{V}_L) \\ = -\nabla \cdot (f_S \mathbf{F}_S + f_L \mathbf{F}_L). \end{aligned} \quad (1)$$

Function $f_{\mathcal{P}}$ denotes the temperature dependent volume fraction, $h_{\mathcal{P}}$ the specific enthalpy, $\mathbf{V}_{\mathcal{P}}$ the known velocity, and $\mathbf{F}_{\mathcal{P}}$ the heat flux of phase \mathcal{P} . Since only two phases are present in the system, $f_S + f_L = 1$. Due to the local thermal equilibrium between the phases, the phase temperatures are equal and represented by T . The phase change takes place between solidus T_S and liquidus temperature T_L . Mean phase change temperature $T_{\mathcal{M}}$ and phase change interval $T_{\mathcal{L}S}$ are

$$T_{\mathcal{M}} = \frac{1}{2} T_S + \frac{1}{2} T_L, \quad T_{\mathcal{L}S} = T_L - T_S. \quad (2)$$

Pure substances are modelled by a suitable narrow phase change interval with $T_{\mathcal{M}}$ in this case standing for melting temperature. Constitutive equations for the two heat fluxes are based on the Fourier relation

$$\mathbf{F}_S = -k_S \nabla T, \quad \mathbf{F}_L = -k_L \nabla T, \quad (3)$$

and the enthalpy-temperature relationships are constituted as

$$h_S = \int_{T_{ref}}^T c_{pS}(\theta) d\theta, \quad h_L = h_S(T_S) + \int_{T_S}^T c_{pL}(\theta) d\theta + h_M, \quad (4)$$

with T_{ref} representing the enthalpy reference temperature. The governing equation could be rewritten in the following latent heat source term form

$$\rho_0 c \frac{\partial T}{\partial t} + \Phi_f \cdot \nabla f_L + \Phi_T \cdot \nabla T + \Phi^f f_L + \Phi^0 = \nabla \cdot (k \nabla T) - \rho_0 h_{LS} \frac{df_L}{dt}. \quad (5)$$

Specific heat c and thermal conductivity k of the continuum are defined as

$$\rho_0 c = f_S h_S \frac{d\rho_S}{dT} + f_L h_L \frac{d\rho_L}{dT} + f_S \rho_S c_{pS} + f_L \rho_L c_{pL}, \quad k = f_S k_S + f_L k_L, \quad (6)$$

the enthalpy difference h_{LS} and the representative density ρ_0 of the system are

$$\rho_0 h_{LS} = \rho_L h_L - \rho_S h_S, \quad \rho_0 = \frac{1}{2} \rho_S(T_M) + \frac{1}{2} \rho_L(T_M). \quad (7)$$

Calculation of the divergence in the convective term gives

$$\Phi \equiv \nabla \cdot (f_S \rho_S h_S \mathbf{V}_S + f_L \rho_L h_L \mathbf{V}_L) = \Phi_f \cdot \nabla f_L + \Phi_T \cdot \nabla T + \Phi^f f_L + \Phi^0, \quad (8)$$

where

$$\begin{aligned} \Phi_f &= \rho_L h_L \mathbf{V}_L - \rho_S h_S \mathbf{V}_S, \\ \Phi_T &= (1 - f_L) \left(\frac{d\rho_S}{dT} h_S + \rho_S c_{pS} \right) \mathbf{V}_S + f_L \left(\frac{d\rho_L}{dT} h_L + \rho_L c_{pL} \right) \mathbf{V}_L, \\ \Phi^f &= \rho_L h_L \nabla \cdot \mathbf{V}_L - \rho_S h_S \nabla \cdot \mathbf{V}_S, \quad \Phi^0 = \rho_S h_S \nabla \cdot \mathbf{V}_S. \end{aligned} \quad (9)$$

We seek the solution of the governing equation for thermal field at final time $t = t_0 + \Delta t$, where t_0 represents initial time and Δt the positive time increment. The solution is constructed by the initial and boundary conditions that follow. The initial temperature $T(\mathbf{p}, t_0)$ at point with position vector \mathbf{p} and time t_0 is defined through the known function T_0

$$T(\mathbf{p}, t_0) = T_0; \quad \mathbf{p} \in \Omega \cup \Gamma. \quad (10)$$

The boundary Γ is divided into not necessarily connected parts Γ^D , Γ^N , and Γ^R

$$\Gamma = \Gamma^D \cup \Gamma^N \cup \Gamma^R, \quad (11)$$

with Dirichlet, Neumann, and Robin type boundary conditions respectively. These boundary conditions are at point \mathbf{p} and time $t_0 \leq t \leq t_0 + \Delta t$ defined through known functions T_Γ , F_Γ , and \mathcal{H}_Γ

$$T(\mathbf{p}, t) = T_\Gamma; \quad \mathbf{p} \in \Gamma^D, \quad (12)$$

$$\frac{\partial T}{\partial n_\Gamma}(\mathbf{p}, t) = -\frac{F_\Gamma}{k}; \quad \mathbf{p} \in \Gamma^N, \quad (13)$$

$$\frac{\partial T}{\partial n_\Gamma}(\mathbf{p}, t) = -\frac{\mathcal{H}_\Gamma}{k} (T - T_\Gamma); \quad \mathbf{p} \in \Gamma^R, \quad (14)$$

where the heat transfer coefficient \mathcal{H}_Γ and other known functions are allowed to depend arbitrarily on the thermal field. The outward pointing normal on Γ is denoted by $\mathbf{n}_\Gamma(\mathbf{p})$. Equation (5) is rewritten by introducing the Kirchhoff variable

$$\mathcal{T}(T) = T_T + \int_{T_T}^T \frac{k(\theta)}{k_0} d\theta, \quad (15)$$

defined with representative thermal conductivity

$$k_0 = \frac{1}{2} k_S(T_M) + \frac{1}{2} k_L(T_M), \quad (16)$$

and with the Kirchhoff variable reference temperature T_T . Knowledge of the inverse Kirchhoff function $T = T(\mathcal{T})$ is assumed as well. The governing equation is accordingly reformulated as

$$\rho_0 k_0 \frac{c}{k} \frac{\partial}{\partial t} \mathcal{T} + \Phi_f \cdot \nabla f_{\mathcal{L}} + \frac{k_0}{k} \Phi_T \cdot \nabla \mathcal{T} + \Phi^f f_{\mathcal{L}} + \Phi^0 = k_0 \nabla^2 \mathcal{T} - \rho_0 h_{\mathcal{L}S} \frac{\partial}{\partial t} f_{\mathcal{L}} \quad (17)$$

and initial and boundary conditions as

$$\begin{aligned} \mathcal{T}(\mathbf{p}, t_0) &= \mathcal{T}(T_0); \quad \mathbf{p} \in \Omega, \\ \mathcal{T}(\mathbf{p}, t) &= \mathcal{T}(T_\Gamma); \quad \mathbf{p} \in \Gamma^D, \\ \frac{\partial \mathcal{T}}{\partial n_\Gamma}(\mathbf{p}, t) &= -\frac{F_\Gamma}{k_0}; \quad \mathbf{p} \in \Gamma^N, \\ \frac{\partial \mathcal{T}}{\partial n_\Gamma}(\mathbf{p}, t) &= -\frac{\mathcal{H}_\Gamma}{k_0} (\mathcal{T}(\mathcal{T}) - T_\Gamma); \quad \mathbf{p} \in \Gamma^R. \end{aligned} \quad (18)$$

The transformed equation (17) with transformed initial and boundary conditions (18) is solved for

$$\frac{\partial \mathcal{T}}{\partial n_\Gamma}(\mathbf{p}, t_0 + \Delta t); \quad \mathbf{p} \in \Gamma^D, \quad \mathcal{T}(\mathbf{p}, t_0 + \Delta t); \quad \mathbf{p} \in \Omega \cup \Gamma^N \cup \Gamma^R, \quad (19)$$

giving the required thermal field through the inverse Kirchhoff function.

3. Discretization

3.1 Time discretization

Time discretization is performed with Crank-Nicolson time differencing

$$\begin{aligned} &\rho_0 k_0 \left(\frac{c}{k}\right)^{j+1/2} \frac{1}{\Delta t} (\mathcal{T}^{j+1} - \mathcal{T}^j) + \frac{1}{2} \Phi_f^{j+1/2} \cdot (\nabla f_{\mathcal{L}}^{j+1} + \nabla f_{\mathcal{L}}^j) \\ &+ \left(\frac{k_0}{k} \Phi_T\right)^{j+1/2} \cdot (\nabla \mathcal{T}^{j+1} + \nabla \mathcal{T}^j) + \frac{1}{2} \Phi^f{}^{j+1/2} (f_{\mathcal{L}}^{j+1} + f_{\mathcal{L}}^j) + \Phi^0{}^{j+1/2} \\ &= \frac{1}{2} k_0 (\nabla^2 \mathcal{T}^{j+1} + \nabla^2 \mathcal{T}^j) - \rho_0 h_{\mathcal{L}S} \frac{1}{\Delta t} (f_{\mathcal{L}}^{j+1} - f_{\mathcal{L}}^j), \end{aligned} \quad (20)$$

where indexes j , $j+1/2$ and $j+1$ represent values at t_0 , $t_0 + \frac{1}{2}\Delta t$ and $t_0 + \Delta t$ respectively. Since liquid volume fraction and other material properties depend on temperature, iterations over the timestep are inherently required in order to find the solution. These iterations are stopped when the maximum absolute value of the enthalpy difference between two successive iterations in each of the gridpoints does not exceed some predetermined value. Updating of the liquid volume fraction is of the utmost importance and various schemes have been used in the past. We adopt the general source-based scheme (Voller et al.[10]) which is believed to be the most effective choice. It is applied to the integral equation concept and the Kirchhoff variable concept and extended to a convective term in this work. The liquid volume fraction at iteration level $m+1$ is approximated with the Kirchhoff variable at iteration level $m+1$ (Voller-Swaminathan einsatz)

$${}^{m+1}f_{\mathcal{L}}^{j+1} = {}^m f_{\mathcal{L}}^{j+1} + m \left(\frac{k_0}{k} \frac{df_{\mathcal{L}}}{dT} \right)^{j+1} ({}^{m+1}\mathcal{T}^{j+1} - \mathcal{T}({}^m f_{\mathcal{L}}^{j+1})). \quad (21)$$

Thermal conductivity and the derivative in the upper equation are evaluated as

$${}^m k^{j+1} = k(T({}^m \mathcal{T}^{j+1})), \quad {}^m \frac{df_{\mathcal{L}}}{dT}{}^{j+1} = \frac{df_{\mathcal{L}}}{dT}({}^m f_{\mathcal{L}}^{j+1}), \quad (22)$$

and $\mathcal{T}({}^m f_{\mathcal{L}}^{j+1})$ stands for $\mathcal{T}(T({}^m f_{\mathcal{L}}^{j+1}))$. By inserting the liquid volume fraction expansion (21) in equation (20) at iteration level $m+1$, the final time-discretized form of equation (17) is obtained.

3.2 Space Discretization

Space discretization is made by weighting the time-discretized equation (17) over domain Ω by the fundamental solution of the Laplace equation T^* . The following integral types are subsequently obtained (\mathcal{F} stands for arbitrary scalar and \mathcal{G} for arbitrary vector valued function respectively)

$$\mathcal{I}_1 = \int_{\Omega} \nabla^2 \mathcal{F}(\mathbf{p}) T^*(\mathbf{p}; \mathbf{s}) d\Omega,$$

$$\mathcal{I}_2 = \int_{\Omega} \mathcal{F}(\mathbf{p}) T^*(\mathbf{p}; \mathbf{s}) d\Omega, \quad \mathcal{I}_3 = \int_{\Omega} \mathcal{G}(\mathbf{p}) \cdot \nabla \mathcal{F}(\mathbf{p}) T^*(\mathbf{p}; \mathbf{s}) d\Omega. \quad (23)$$

Let us focus on two dimensional situations, e.g.

$$T^*(\mathbf{p}; \mathbf{s}) = \frac{1}{2\pi} \log \frac{r_0}{r}; \quad r^2 = (\mathbf{p} - \mathbf{s}) \cdot (\mathbf{p} - \mathbf{s}), \quad (24)$$

with the simplest boundary discretization; boundary geometry is approximated by N_F straight line segments, and spatial variation of the fields on each of the boundary segments is represented by constant interpolation functions with gridpoints coinciding with the geometrical centers of the straight line

segments. Spatial variation of the fields in Ω is represented by the global interpolation functions of the form (Einstein summation convention is used in this text)

$$\mathcal{F}(\mathbf{p}) \approx \psi_u(\mathbf{p}) \zeta_u; \quad u=1,2,\dots,N+3. \quad (25)$$

Selection of thin plate splines (Golberg et al.[11]) for ψ_u gives an optimal approximating property. The two-dimensional form of these splines is

$$\psi_n(\mathbf{p}) = r_n^2 \log r_n; \quad n=1,2,\dots,N, \quad \psi_{N+1}(\mathbf{p}) = p_x, \quad \psi_{N+2}(\mathbf{p}) = p_y, \quad \psi_{N+3}(\mathbf{p}) = 1, \\ r_n^2 = (\mathbf{p} - \mathbf{p}_n) \cdot (\mathbf{p} - \mathbf{p}_n), \quad p_x = \mathbf{p} \cdot \mathbf{i}_x, \quad p_y = \mathbf{p} \cdot \mathbf{i}_y, \quad (26)$$

where \mathbf{i}_x and \mathbf{i}_y represent the Cartesian base vectors. ζ_u coefficients are calculated by constructing a system of $N+3$ algebraic equations

$$\Psi \boldsymbol{\zeta} = \mathcal{F}. \quad (27)$$

The vectors are $\boldsymbol{\zeta} = (\zeta_1, \zeta_2, \dots, \zeta_{N+3})^t$ and $\mathcal{F} = (\mathcal{F}_1, \mathcal{F}_2, \dots, \mathcal{F}_N, 0, 0, 0)^t$. The first $v=1,2,\dots,N$ rows of matrix Ψ are of the form $(\psi_{v1}, \psi_{v2}, \dots, \psi_{vN+3})$, and the last three rows $v=N+1, N+2, N+3$ are of the form $(\psi_{1v}, \psi_{2v}, \dots, \psi_{Nv}, 0, 0, 0)$, where the notation has been shortened to $\mathcal{F}_n \equiv \mathcal{F}(\mathbf{p}_n)$, $\psi_{nu} \equiv \psi_u(\mathbf{p}_n)$. The first N_Γ points \mathbf{p}_n coincide with the boundary gridpoints and the last N_Ω points are arbitrarily distributed over the domain Ω ($N=N_\Gamma+N_\Omega$). ζ_u coefficients follow by inverting the system (27)

$$\boldsymbol{\zeta} = \Psi^{-1} \mathcal{F}. \quad (28)$$

The first integral type could be straightforwardly calculated by using Green's second identity

$$\int_{\Omega} \nabla^2 \mathcal{F} T_l^* d\Omega \approx G_{lk} \delta_{ki} \frac{\partial \mathcal{F}_i}{\partial n_\Gamma} - H_{lk} \delta_{ki} \mathcal{F}_i - c_l^* \delta_{li} \mathcal{F}_i,$$

where $k=1,2,\dots,N_\Gamma$ and $i,l=1,2,\dots,N$. Index l stands for $\mathbf{s}_l = \mathbf{p}_l$. Matrix elements G_{lk} and H_{lk} are defined as follows

$$G_{lk} = \int_{\Gamma_k} T_l^* d\Gamma, \quad H_{lk} = \int_{\Gamma_k} \frac{\partial T_l^*}{\partial n_\Gamma} d\Gamma, \quad (29)$$

where Γ_k represents the k -th boundary segment, and c_l^* is equal to

$$c_l^* = \frac{1}{2}; \quad \mathbf{s}_l \in \Gamma, \quad c_l^* = 1; \quad \mathbf{s}_l \in \Omega. \quad (30)$$

The second and third integral identities are calculated by defining (Partridge et al.[12]) the harmonic functions $\hat{\psi}_u$

$$\nabla^2 \hat{\psi}_u(\mathbf{p}) = \psi_u(\mathbf{p}). \quad (31)$$

The corresponding functions $\hat{\psi}_u$ for the thin plate splines (26) are

$$\hat{\psi}_n = \frac{1}{16} r_n^4 \log r_n - \frac{1}{32} r_n^4, \quad \hat{\psi}_{N+1} = \frac{1}{6} p_x^3, \quad \hat{\psi}_{N+2} = \frac{1}{6} p_y^3, \quad \hat{\psi}_{N+3} = \frac{1}{6} \mathbf{p} \cdot \mathbf{p}. \quad (32)$$

Consequently, the second and third integral types can be written in a compact dual reciprocity form ($k=1,2,\dots,N_\Gamma$, $i,l,o=1,2,\dots,N$, $u,v=1,2,\dots,N+3$)

$$\int_\Omega \mathcal{F} T_l^* d\Omega \approx \Psi_{lu} \Psi_{ui}^{-1} \mathcal{F}_i, \quad \int_\Omega \mathbf{g} \cdot \nabla \mathcal{F} T_l^* d\Omega \approx \Psi_{lu} \Psi_{uo}^{-1} \mathbf{g}_o \cdot \nabla \psi_{ov} \Psi_{vi}^{-1} \mathcal{F}_i,$$

$$\Psi_{lu} \equiv \int_\Omega \nabla^2 \hat{\psi}_u T_l^* d\Omega \approx G_{lk} \delta_{ki} \frac{\partial \hat{\psi}_{iu}}{\partial n_\Gamma} - H_{lk} \delta_{ki} \hat{\psi}_{iu} - c_l^* \delta_{li} \hat{\psi}_{iu}. \quad (33)$$

3.3 Final discretized expression

After weighting the time discretized governing equation by the fundamental solution of the Laplace equation and calculating the boundary and domain integrals as described, the following discretized form is structured

$$\left({}^m F_{li}^{j+1} + {}^m F_{cli}^{j+1} \right) m^{+1} \mathcal{T}_i^{j+1} + {}^m T_{li}^{j+1} m^{+1} \frac{\partial \mathcal{T}_i^{j+1}}{\partial n_\Gamma}$$

$$= \left({}^m F_{li}^j + {}^m F_{cli}^j \right) \mathcal{T}_i^j + \left({}^m T_{li}^j + {}^m T_{cli}^j \right) \frac{\partial \mathcal{T}_i^j}{\partial n_\Gamma} + {}^m D_l + {}^m D_{cl}, \quad (34)$$

where the coefficients F_c , T_c , and D_c arise from the discretized convective term and the coefficients F , T and D from all other discretized terms of equation (17). The explicit forms of the coefficients in equation (34) are

$${}^m F_{li}^{j+1} = \Psi_{lu} \Psi_{ui}^{-1} \left(\rho_0 k_0 m \left(\frac{c}{k} \right)_i^{j+1/2} \frac{1}{\Delta t} + \rho_0 {}^m h_{\mathcal{L}Si}^{j+1/2} m \left(\frac{k_0}{k} \frac{\partial f_{\mathcal{L}}}{\partial T} \right)_i^{j+1} \frac{1}{\Delta t} \right)$$

$$+ k_0 \frac{1}{2} \left(H_{lk} \delta_{ki} + c_l^* \delta_{li} \right), \quad (35)$$

$${}^m T_{li}^{j+1} = -k_0 \frac{1}{2} G_{lk} \delta_{ki}, \quad (36)$$

$${}^m F_{li}^j = \Psi_{lu} \Psi_{ui}^{-1} \left(\rho_0 k_0 m \left(\frac{c}{k} \right)_i^{j+1/2} \frac{1}{\Delta t} \right) - k_0 \frac{1}{2} \left(H_{lk} \delta_{ki} + c_l^* \delta_{li} \right), \quad (37)$$

$${}^m T_{li}^j = +k_0 \frac{1}{2} G_{lk} \delta_{ki} \quad (38)$$

$${}^m D_l = -\Psi_{lu} \Psi_{ui}^{-1} \left(\rho_0 {}^m h_{\mathcal{L}Si}^{j+1/2} \frac{1}{\Delta t} \left({}^m f_{\mathcal{L}i}^{j+1} - f_{\mathcal{L}i}^j \right) \right.$$

$$\left. - \rho_0 {}^m h_{\mathcal{L}Si}^{j+1/2} m \left(\frac{k_0}{k} \frac{\partial f_{\mathcal{L}}}{\partial T} \right)_i^{j+1} \frac{1}{\Delta t} \mathcal{T} \left({}^m f_{\mathcal{L}i}^{j+1} \right) \right), \quad (39)$$

$$\begin{aligned}
 {}^m F_{cli}^{j+1} = & \frac{1}{2} \left[\Psi_{lu} \Psi_{uo}^{-1} m \left(\frac{k_0}{k} \Phi_T \right)_o^{j+1/2} \cdot \nabla \psi_{\underline{ov}} \Psi_{vi}^{-1} \right. \\
 & + \Psi_{lu} \Psi_{uo}^{-1} m \Phi_{fo}^{j+1/2} \cdot \nabla \psi_{\underline{ov}} \Psi_{vi}^{-1} m \left(\frac{k_0}{k} \frac{df_{\mathcal{L}}}{dT} \right)_i^{j+1} \\
 & \left. + \Psi_{lu} \Psi_{ui}^{-1} m \Phi_i^{f, j+1/2} m \left(\frac{k_0}{k} \frac{df_{\mathcal{L}}}{dT} \right)_i^{j+1} \right], \quad (40)
 \end{aligned}$$

$${}^m F_{cli}^j = -\frac{1}{2} \Psi_{lu} \Psi_{uo}^{-1} m \left(\frac{k_0}{k} \Phi_T \right)_o^{j+1/2} \cdot \nabla \psi_{\underline{ov}} \Psi_{vi}^{-1}, \quad (41)$$

$$\begin{aligned}
 {}^m D_{cl} = & -\Psi_{lu} \Psi_{ui}^{-1} m \Phi_i^{0, j+1/2} \\
 & -\frac{1}{2} \Psi_{lu} \Psi_{uo}^{-1} m \Phi_{fo}^{j+1/2} \cdot \nabla \psi_{\underline{ov}} \Psi_{vi}^{-1} \left(m f_{\mathcal{L}i}^{j+1} + f_{\mathcal{L}i}^j - m \left(\frac{k_0}{k} \frac{df_{\mathcal{L}}}{dT} \right)_i^{j+1} \mathcal{T}(m f_{\mathcal{L}i}^{j+1}) \right) \\
 & -\frac{1}{2} \Psi_{lu} \Psi_{ui}^{-1} m \Phi_i^{f, j+1/2} \left(m f_{\mathcal{L}i}^{j+1} + f_{\mathcal{L}i}^j - m \left(\frac{k_0}{k} \frac{df_{\mathcal{L}}}{dT} \right)_i^{j+1} \mathcal{T}(m f_{\mathcal{L}i}^{j+1}) \right). \quad (42)
 \end{aligned}$$

The divergence of the velocity fields $\mathbf{V}_{\mathcal{P}}$ in the convective term coefficients Φ^f and Φ^0 is calculated as

$$\nabla \cdot \mathbf{V}_{\mathcal{P}i} = \frac{\partial \psi_{iu}}{\partial x} \Psi_{un}^{-1} V_{\mathcal{P}xn} + \frac{\partial \psi_{iu}}{\partial y} \Psi_{un}^{-1} V_{\mathcal{P}yn}. \quad (43)$$

Rearrangement of the matrix elements (34) with respect to the boundary conditions gives a system of algebraic equations for solving the unknowns ${}^{m+1}\mathcal{T}_n^{j+1}$ or ${}^m \frac{\partial \mathcal{T}^{j+1}}{\partial n_{\Gamma_n}}$ on the boundary and ${}^{m+1}\mathcal{T}_n^{j+1}$ in the domain.

4. Liquid volume fraction updating strategy

After calculation of the Kirchhoff variable at time $j+1$ and iteration $m+1$, the liquid volume fraction has to be updated. We distinguish two different cases, the first one with liquid volume fraction in the phase-change interval $0 < m f_{\mathcal{L}}^{j+1} < 1$ and the second one with liquid volume fraction outside the phase change interval ${}^m f_{\mathcal{L}}^{j+1} = 1$, or ${}^m f_{\mathcal{L}}^{j+1} = 0$. In the first case, the liquid volume fraction is updated directly from equation (21). In the second case, the derivative ${}^m \frac{df_{\mathcal{L}}}{dT}^{j+1}$ equals zero and melting or solidification processes can not be started when using the above-mentioned formula. A suitable updating strategy for such cases is derived as follows. The time discretized expression (20) for evaluation of the Kirchhoff variable at iteration level $m+1$ is written in the following simplified form

$${}^m A {}^{m+1} \mathcal{T}^{j+1} = {}^m B - \rho_0 {}^m h_{\mathcal{L}S}^{j+1/2} \frac{1}{\Delta t} ({}^m f_{\mathcal{L}}^{j+1} - f_{\mathcal{L}}^j), \quad (44)$$

where the coefficient ${}^m A$ stands for ${}^m A = \rho_0 k_0 m \left(\frac{c}{k}\right)^{j+1/2} \frac{1}{\Delta t}$, and the term ${}^m B$ for all other terms not explicitly represented in equation (44). At convergence, the following expression should be valid

$${}^{m+1} A \mathcal{T}({}^{m+1} f_{\mathcal{L}}^{j+1}) = {}^{m+1} B - \rho_0 {}^{m+1} h_{\mathcal{L}S}^{j+1/2} \frac{1}{\Delta t} ({}^{m+1} f_{\mathcal{L}}^{j+1} - f_{\mathcal{L}}^j). \quad (45)$$

In equation (45), the Kirchhoff variable is expanded as

$${}^{m+1} \mathcal{T}^{j+1} = \mathcal{T}({}^m f_{\mathcal{L}}^{j+1}) + m \left(\frac{k}{k_0} \frac{dT}{df_{\mathcal{L}}} \right)^{j+1} ({}^{m+1} f_{\mathcal{L}}^{j+1} - {}^m f_{\mathcal{L}}^{j+1}) \quad (46)$$

and equation (45) is subtracted from equation (44), assuming ${}^{m+1} B \approx {}^m B$, and ${}^{m+1} A \approx {}^m A$. This gives the second updating formula

$${}^{m+1} f_{\mathcal{L}}^{j+1} = {}^m f_{\mathcal{L}}^{j+1} + \left(\frac{{}^m h_{\mathcal{L}S}^{j+1/2}}{k_0 m \left(\frac{c}{k}\right)^{j+1/2}} + m \left(\frac{k}{k_0} \frac{dT}{df_{\mathcal{L}}} \right)^{j+1} \right)^{-1} ({}^{m+1} \mathcal{T}^{j+1} - \mathcal{T}({}^m f_{\mathcal{L}}^{j+1})). \quad (47)$$

Material properties c and k and the derivative are calculated in the same sense as described in equation (22). Note that thermal conductivity is calculated at times $j+1/2$ and $j+1$. Since expressions (21,47) could give physically impossible liquid volume fractions (less than 0 or greater than 1), each updating is corrected (Voller et al.[10]) by the over/undershoot formula

$${}^{m+1} f_{\mathcal{L}}^{j+1} > 1 : \text{ set } {}^{m+1} f_{\mathcal{L}}^{j+1} = 1, \quad {}^{m+1} f_{\mathcal{L}}^{j+1} < 0 : \text{ set } {}^{m+1} f_{\mathcal{L}}^{j+1} = 0. \quad (48)$$

5. Conclusions

The principal advantage of the described procedure is the ease of coping with geometrically complicated situations, ease of implementation of different boundary condition types, same order of temperature and heat flux approximation at the boundary, accuracy, and simple mesh structure. All integrations involved are carried out on the boundary-only basis. The method is extremely robust since no heuristic parameters are required to update the liquid volume fraction or over/under relax a broad spectra of realistic (Šarler [to appear]) temperature dependent material properties during computations. The main disadvantage of the method remains the resulting large asymmetrical algebraic system of equations and relatively involved calculation of the domain integrals (particularly the \mathcal{I}_3 integral) by the finite set of boundary integrals, since the domain gridpoints are inherently required in solving the described class of highly non-linear problems.

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