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Numerical Solutions of Multi-Dimensional Solidification/Melting Problems by the Dual Reciprocity Boundary Element Method

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Abstract

This paper presents an effective and simple procedure for the simulation of the motion of the solid-liquid interfacial boundary and the transient temperature field during phase change process. To accomplish this purpose, an iterative implicit solution algorithm has been developed by employing the dual reciprocity boundary element method. The dual reciprocity boundary element approach provided in this paper is much simpler than the usual boundary element method applying a reciprocity principle and an available technique for dealing with domain integral of boundary element formulation simultaneously. The effectiveness of the present analysis method have been illustrated through comparisons of the calculation results of an example with its semi-analytical or other numerical solutions where available.

I. Introduction

Transient heat transfer problems with phase changes (Stefan problems) occur in many engineering situations, including potential core melting and solidification during pressurized water reactor severe accidents, ablation of thermal shields and many others. Such problems are inherently nonlinear due to the condition on the interfacial moving boundary, resulting in significant theoretical difficulties. Thus various numerical methods such as finite differences, finite elements, finite volumes or boundary elements[1] have been proposed to deal with those problems. Since one-dimensional Stefan problem was studied with the boundary element method(BEM) by Shaw[2] and Wrobel[3], many investigators[4-12] dealt with two-dimensional BEM formulations for the Stefan problem as quasi-static. However, their approach lacks in generality and introduces further approximations compromising the accuracy of the results. O'Neill[13] gave a general integral formulation for quasi-static phase problems. Zabaras and Mukherjee[14,15] and Delima-Silva Jr. and Wrobel[16-18] extended the works of O'Neill[13] to two-dimensional transient problems in different articles using convolution-type integrals.

This paper presents a dual reciprocity boundary element (DRBEM) formulation for multi-dimensional heat transfer problems either with solidification or melting process, using a time-dependent fundamental solution and a predictor-corrector iterative scheme for tracking the moving solid-liquid interfacial boundary [18]. The DRBEM formulation for the Stefan problems presented in this paper does not involve any integral terms, thus resulting in easier numerical implementation. The effectiveness of the present method is examined by comparing the calculation results with the existing solutions for some examples where available.

II. Mathematical Formulation for Multi-Dimensional Solidification/Melting Problems

Consider a situation that a liquid at an initially uniform temperature T_i (equal to or above the melting point T_m), occupying a region with a fixed boundary Γ_o, is cooled to a temperature lower than the melting point by heat exchange at the outer boundary Γ_o with an environmental medium as shown in Fig. 1-a. Initially, solidification of the liquid starts all around the outer boundary Γ_o and the interfacial boundary Γ_I between the solid and liquid phases is moving inwards as the latent heat of fusion is liberated. In similar manner let's consider another situation that a solid at an initially uniform temperature T_i (below the melting point T_m), forming a region with a fixed boundary Γ_o, is heated up to the melting temperature by heat exchange at the outer boundary Γ_o with an environmental medium as shown in Fig. 1-b. In this case, as the heating progresses , eventually the outer boundary Γ_o reaches the phase change temperature and melting of the solid starts all around the boundary Γ_o, and then the interfacial boundary Γ_I between the liquid and solid phases is moving inwards as the latent heat of fusion is absorbed.

Assuming Constant material parameters and no motion of liquid, the governing differential equations for both cases can be expressed as follows:

$$\nabla^2 T_s(\mathbf{x},t) + \frac{1}{k_s} g_s(\mathbf{x},t) = \frac{1}{a_s}\frac{\partial T_s(\mathbf{x},t)}{\partial t}, \quad \mathbf{x} \in \Omega_s(t) \tag{1}$$

$$\nabla^2 T_\ell(\mathbf{x},t) + \frac{1}{k_\ell} g_\ell(\mathbf{x},t) = \frac{1}{a_\ell}\frac{\partial T_\ell(\mathbf{x},t)}{\partial t}, \quad \mathbf{x} \in \Omega_\ell(t) \tag{2}$$

where the subscripts s and ℓ are used to stand for the solid and liquid phases, respectively, $\Omega_s(t)$ denotes the solid domain at time t, $T_s(\mathbf{x},t)$ is the temperature at the point $\mathbf{x} \in \Omega_s(t)$, $g_s(\mathbf{x},t)$ is the rate of heat generation in the solid region at time t, $\mathbf{x}$ contains the cartesian coordinates x, y and z, and k and a are the thermal conductivity and thermal diffusivity, respectively. Similar definitions are applied to $T_\ell(\mathbf{x},t)$ and $g_\ell(\mathbf{x},t)$ for the liquid region. The thermal diffusivities a_s and a_ℓ are equal to $k_s/\rho_s c_s$ and $k_\ell/\rho_\ell c_\ell$, respectively, where ρ and c are density and specific heat, respectively. The initial, boundary and freezing (moving) interface conditions are given as

	$\Omega_s = 0$ and $\Omega_\ell = \Omega_w$	$at\ t=0$ where $\Omega_w = \Omega_s(t) + \Omega_\ell(t)$	(3a)
	$T(\mathbf{x},o) = T_i = const.$	for $\mathbf{x} \in \Omega_\ell(o)$ in case of solidification	(3b-1)
or		for $\mathbf{x} \in \Omega_s(o)$ in case of melting	(3b-2)
	$T(\mathbf{x},t) = T_o(\mathbf{x},t)$	for $\mathbf{x} \in \Gamma_{01}(t)$	(3c)
	$q(\mathbf{x},t) = q_o(\mathbf{x},t)$	for $\mathbf{x} \in \Gamma_{02}(t)$	(3d)
	$T(\mathbf{x},t) = T_m$	for $\mathbf{x} \in \Gamma_I(t)$	(3e)
	$k_s \frac{\partial T_s}{\partial n_s} - k_\ell \frac{\partial T_\ell}{\partial n_s} = \rho_s L V_n$	for $\mathbf{x} \in \Gamma_I(t)$ in case of solidification	(3f-1)
or	$k_\ell \frac{\partial T_\ell}{\partial n_s} - k_s \frac{\partial T_s}{\partial n_s} = \rho_s L V_n$	for $\mathbf{x} \in \Gamma_I(t)$ in case of melting	(3f-2)

where the subscript I indicates the solid-liquid interface, T_o is a prescribed transient temperature distribution on the part Γ_{01} of the whole boundary Γ_w $(=\Gamma_{01}+\Gamma_{02}+\Gamma_I)$ and q_o is the prescribed heat flux being resulted from convective and/or radiative heat transfer on the remaining part Γ_{02} of Γ_w, L is the latent heat of fusion, n is the outward normal direction

and V_n is the normal outward velocity at a point $\mathbf{x}$ on the moving (freezing) boundary defined as $$V_n = \frac{\partial \mathbf{x}(t)}{\partial t} \cdot \mathbf{n}_u \tag{4}$$
where $\mathbf{x}(t) = x(t)\,\mathbf{i} + y(t)\,\mathbf{j} + z(t)\,\mathbf{k}$ is location history of a point on the moving boundary $\Gamma_f(t)$ defined in terms of unit vectors $(\mathbf{i}, \mathbf{j}, \mathbf{k})$ along the global Cartesian axes, and $\mathbf{n}_u$ is the unit normal vector on the moving boundary $\Gamma_f(t)$ at a point $\mathbf{x} \in \Gamma_f(t)$, pointing outwards from the solid region.

III. Dual Reciprocity Boundary Element Formulation

For the dual reciprocity boundary element method(DRBEM) solutions for the temperature fields in the solid and liquid phase regions, Eqs.(1) and (2) can be written in the generalized form as $$\nabla^2 T_p(\mathbf{x}, t) = \frac{1}{\alpha_p}\left[\,\dot{T}_p(\mathbf{x}, t) - \frac{\alpha_p}{k_p} g_p(\mathbf{x}, t)\right],\ \ \mathbf{x} \in \Omega_p,\ \ p = s, \ell \tag{5}$$
where the dot stands for the time derivative, and the subscript p represents the subscripts s and ℓ which are used to indicate the solid and liquid phases, respectively. Hereafter, the subscript p is omitted for simplicity.

Applying the usual boundary element technique, based on the use of the fundamental solution and reciprocity principle (Green's theorem) to Eq.(5), the following integral equation can be deduced.

$$C_i T_i + \int_\Gamma T q^* d\Gamma - \int_\Gamma q T^* d\Gamma = \int_\Omega \frac{1}{\alpha}\left(\dot{T} - \frac{\alpha}{k} g\right) T^* d\Omega \tag{6}$$

where T^* and q^* are the fundamental solutions of Poisson equation, representing the field generated by a concentrated unit source acting at a point i.

The key idea of DRBEM is to take the remaining domain integral term to the boundary with the use of the reciprocity principle once again for removing the need for complicated domain discretization. To accomplish this purpose, first, the source-like term of Eq.(5) is approximated by utilizing the method of a separation of variables as

$$\frac{1}{\alpha}\left(\dot{T} - \frac{\alpha}{k} g\right) \simeq \sum_{j=1}^{N+L} f_j(\mathbf{x})\beta_j(t) \tag{7}$$

where $\beta_j(t)$ are a set of initially unknown functions of time, $f_j(\mathbf{x})$ are known function of geometry, and N and L are the numbers of boundary and internal nodes, respectively.

And then, the approximating functions $f_j(\mathbf{x})$ and the particular solutions $\hat{T}_j$ is linked through the relation, $$\nabla^2 \hat{T}_j = f_j \tag{8}$$

Substituting Eqs.(7) and (8) into Eq.(6), and applying integration by parts two times to the domain integral term of Eq.(6) gives

$$C_i T_i + \int_\Gamma q^* T\, d\Gamma - \int_\Gamma T^* q\, d\Gamma = \sum_{j=1}^{N+L} \beta_j \left(C_i \hat{T}_{ij} + \int_\Gamma q^* \hat{T}_j\, d\Gamma - \int_\Gamma T^* \hat{q}_j\, d\Gamma\right) \tag{9}$$

where $\hat{q}_j$ is defined as $\hat{q}_j = \partial \hat{T}_j / \partial n$, and n is the unit outward normal to Γ_o.

Assuming that the whole boundary of any domain of interest is divided into N elements, Eq.(9) can be written in a discretized form, with summations over the boundary elements replacing the integrals. Thereafter the use of a collocation technique leads to the resultant equation in a matrix form as

$$HT - Gq = (H\hat{T} - G\hat{q})\beta \tag{10}$$

where H and G respectively are matrices of their elements H_{ik} and G_{ik} with C_i being incorporated to the principal diagonal of H. The elements H_{ik} and G_{ik} are defined as

$$H_{ik} = \overline{H_{ik}} + C_i\delta_{ik} \ , \quad \overline{H_{ik}} = h^2_{i(k-1)} + h^1_{ik}, \qquad G_{ik} = g^2_{i(k-1)} + g^1_{ik} \tag{11}$$

where δ_{ik} is the Kronecker delta and

$$h^1_{ik} = \int_{\Gamma_k} \phi_1 q^* d\Gamma \ , \ h^2_{ik} = \int_{\Gamma_k} \phi_2 q^* d\Gamma \ , \ g^1_{ik} = \int_{\Gamma_k} \phi_1 T^* d\Gamma \ , \ g^2_{ik} = \int_{\Gamma_k} \phi_2 T^* d\Gamma \ , \quad h^2_{i0} = h^2_{iN}, \ g^2_{i0} = g^2_{iN} \tag{12}$$

, and where the first and second indices of dual subscripts indicate the specified position of the point where the evaluation is performed and the boundary element over which the contour integration is carried out, respectively, and the superscripts 1 and 2 respectively are used to identify the linear interpolation functions ϕ_1 and ϕ_2 with which the T^* and q^* functions are weighted in the integral terms. The matrices T, q, $\hat{T}$, and q of Eq.(10) correspond to vectors T_k, q_k, T_{kj} and q_{kj}, respectively, and the vector β is defined as

$$\beta = \frac{1}{a} F^{-1} (\dot{T} - \frac{a}{k} g) \tag{13}$$

where F^{-1} is the inverse matrix of F which consists of a vector f_j containing the values of the function f_j at the $(N+L)$ DRBEM collocation points, and $\dot{T}$ and g are the time derivative of the matrix T and the heat source term matrix, respectively.

Substituting Eq.(13) into Eq.(12), the following expression is obtained

$$C\dot{T} + HT = Gq + CS \tag{14}$$

where

$$C = -\frac{1}{a} (H\hat{T} - G\hat{q}) F^{-1} \quad , \qquad S = \frac{a}{k} g \tag{15}$$

IV. Numerical Implementation

Linear approximation in time

For simplicity, a two-level time integration scheme is employed in this study[19]. To do this, a linear approximation for the variation of T and q within each time step is adopted, in the form

$$T = (1-\zeta_T) T^m + \zeta_T T^{m+1} \tag{16}$$

$$q = (1-\xi_q) q^m + \xi_q q^{m+1} \tag{17}$$

$$\dot{T} = \frac{1}{\Delta t} (T^{m+1} - T^m) \tag{18}$$

where ζ_T and ξ_q are parameters, taking the values between 0 and 1, which position the values of T and q, respectively, between time level m and m+1, and Δt denotes a specified time step.

Substituting Eqs.(16)-(18) into Eq.(14) gives as

$$\left(\frac{1}{\Delta t} C + \zeta_T H \right) T^{m+1} - \xi_q \, Gq^{m+1} = \left[\frac{1}{\Delta t} C - (1-\zeta_T) H \right] T^m + (1-\xi_q) \, Gq^m + CS \tag{19}$$

where the right - hand side of Eq.(19) is known at time $(m+1)\Delta t$, because it involves values which have been specified as initial conditions and known functions or calculated at the previous time $m\Delta t$.

As shown above, the major advantages of the DRBEM formulation with respect to other techniques for addressing the Stefan problem come from the facts that meshing is needed only on the boundaries of the solution domain, the problem can be solved for the heat fluxes directly as in the use of usual boundary element method and the DRBEM formulation does not involve any domain integral term.

Moving boundary motion

The normal direction of the node i can be defined by a length weighted average normal vector $\boldsymbol{n}_i$ at the node i as

$$\boldsymbol{n}_i = \frac{\boldsymbol{n}_{j-1}\ell_{j-1} + \boldsymbol{n}_j \ell_j}{\ell_{j-1} + \ell_j} \quad (20)$$

where, the lengths ℓ_{j-1} and ℓ_j and the unit normals $\boldsymbol{n}_{j-1}$ and $\boldsymbol{n}_j$ are for two contiguous boundary elements j-1 and j of the node i. Thus, the unit normal vector $n_{u,i}$, of Eq.(4), along which the normal velocity V_{ni} at the node i is assigned, can be computed by dividing the vector $\boldsymbol{n}_i$, given by Eq.(20), by its own magnitude as follows:

$$\boldsymbol{n}_{u,i} = \frac{\boldsymbol{n}_i}{|\boldsymbol{n}_i|} \quad (21)$$

Now, the new positions of the nodes on the moving boundary can be computed by using the following equation[18]:

$$\mathbf{x}_i^F = \mathbf{x}_i^{F-1} + (V_{navg,i}^{F-1,F} \Delta t_F) \cdot \boldsymbol{n}_{u,i} \quad (22)$$

where $\mathbf{x}_i^F$ and $\mathbf{x}_i^{F-1}$ are the position vectors (containing the cartesian coordinates) of the node i on the moving boundary at a specified time t_F and its previous time t_{F-1}, respectively, the time step Δt_F is equal to $t_F - t_{F-1}$, and $V_{navg,i}^{F-1,F}$ indicates the averaged normal velocity V_{ni} of the node i during the time step Δt_F.

Iteration algorithm

The numerical solution of the nonlinear problem considered here can be obtained by applying an iterative algorithm for addressing the nonlinearity of the problem, originated from the unknown trajectory of the moving interfacial boundary. A general solution algorithm which can be applied for solving one or two-dimensional problems is summarized as

(1) Divide the fixed (outer) boundary of the domain initially occupied either with a liquid or a solid at a uniform temperature into N_0 linear elements.

(2) Assume the initial predicted average velocities of the moving boundary nodes V_{pred}^{avg} at the beginning of the first time step Δt_1.

(3) Calculate the location of the solid-liquid interfacial(moving) boundary based on the assumed values of V_{pred}^{avg}.

(4) Divide the moving boundary into N_I linear elements.

(5) Define interior nodes necessary for obtaining accurate solution both in the solid and liquid phase regions, of which the numbers are L_s and L_ℓ, respectively.

(6) With the known average (predicted) velocity V_{pred}^{avg}, determine the predicted geometry at the end of the time step, then calculate all matrices in Eq.(19) and solve for either T or Q on the fixed and moving boundaries, and finally, compute the new values of V_F^{calc} by using Eqs.(3f) and (4), where V_F^{calc} is the calculated moving boundary velocity at the end of the actual time step after a new iteration.

(7) Determine the corrected average velocity V_{cor}^{avg} from previous time t_{F-1} and current time t_F as $\quad V_{cor}^{avg} = \frac{1}{2}(V_{F-1} + V_F^{calc})$

where V_{F-1} is the moving boundary velocity at the end of the previous time step and

V_{cor}^{avg} is the corrected average velocity of the moving boundary at time step $\triangle t_F$.

(8) Check convergence : If $\dfrac{|V_{cor}^{avg} - V_{pred}^{avg}|}{|V_{cor}^{avg}|} > \varepsilon_{max}$

(where $|\cdot|$ denotes a vector norm and ε_{max} is a pre-specified maximum acceptable error), set $V_{cor}^{avg} = V_{pred}^{avg}$ and continue the operations iteratively from step (6) until the relative error becomes less than or equal to ε_{max}.

(9) If convergence is achieved, update geometry, temperatures and fluxes, and continue to the next time step with $V_{pred}^{avg} = V_F$

where V_F is the moving boundary velocity at the end of the actual time step.

(10) Before updating of geometry and continuation to the next time step, it is necessary to check if the positions of the moving boundary nodes at time t_F, obtained at the end of a successful iteration, could result in numerical instabilities due to the formation of a kink in the boundary or a distorted mesh causing the occurrence of tangling, or nodes coming very close to each other at the next time step $\triangle t_{F+1}$ from t_F to t_{F+1}. When this is the case, remeshing has to be performed at the time t_F, by node removal or node rearrangement as mentioned previously.

V. Numerical Example

To illustrate the validity of the DRBEM technique, presented in this paper, for solving the Stefan problems, some numerical tests have been performed. For this purpose, one example of which the solutions obtained by other methods are available in the literatures[15, 20-22] have been considered in this study. In order to facilitate the comparisons of the present solutions with available data, the following dimensionless parameters have been used :

$$\tilde{\alpha}_s = 1, \quad \tilde{\alpha}_\ell = \frac{\alpha_\ell}{\alpha_s}, \quad \tilde{c}_s = 1, \quad \tilde{c}_\ell = \frac{c_\ell}{c_s}, \quad \tilde{x} = \frac{x}{R}, \quad \tilde{y} = \frac{y}{R}, \quad \tau = \frac{\alpha_s t}{R^2},$$

$$\theta = \frac{T - T_m}{T_m - T_o}, \quad St = \frac{c_s(T_m - T_o)}{L}$$

where R , St and c_s are a characteristic length, the Stefan number and the specific heat of the solid phase, respectively. The values of ζ_T = 1.0 and ξ_q = 1.0 are used for solving Eq.(19) in the present test.

The example is that of a square 2x2 which is initially filled with liquid at the melting temperature ($\theta_i = 0$) and is suddenly subject to a constant surface temperature below the melting point. It is assumed that the liquid has no heat generation for simplicity. As mentioned previously, the major advantage of using the DRBEM for addressing the Stefan problem comes from the facts that meshing is needed only on the boundaries of the solution domain and the problem can be solved for the heat fluxes directly. In this calculations, 32 linear boundary elements for the fixed outer boundary were used and a time step of τ=0.025 was adopted. For the specified maximum relative error of 10^{-3}, the number of iterations, with which convergence was achieved, was 21 in the first starting time step calculation while in all the succeeding time step calculations it varied between a minimum of 4 and a maximum of 19. The remeshing by node removal is adopted to avoid potential numerical instabilities which may be caused by the moving interfacial boundary nodes coming too close.

The DRBEM results are compared on Fig.2 with the BEM-convolution type integral solution of Zabaras and Mukherjee[15], and in Fig.2 with the implicit finite difference solution of Rao and Sastri[20] and the pioneering work of Lazaridis[21], and also with the semi-analytical solution of Rathjen and Jiji[22]. As is seen from the figures, the present DRBEM solutions compare very well with those by other methods.

VI. Conclusions

The DRBEM technique presented in this study, as compared to other numerical methods, has been shown to be very effective and simple to use not only since it has no serious time step limitations and permits the use of relatively coarse and irregular mesh as in the usual BEM formulation for the same problem, but the DRBEM formulation has no integral terms such that the need for evaluating such convolution type integrals as being involved in the usual BEM formulation is removed. The present iterative solution algorithm yielded desirable results such that only a few number of iterations leads to convergence for the specified relative error of 10^{-3} in all the cases tested here. It is seen from the calculation results of the tests investigated in this study that the DRBEM solutions are in good agreement with the existing analytical or numerical solutions.

It is emphasized that the DRBEM solutions of nonlinear transient heat transfer problems involving heat generation within the solution domain, which have been formulated in this study, can be as well computed with little difficulty by following the similar numerical implementation procedure. Consequently, the method presented is considered to be very promising for a variety of nonlinear transient heat transfer problems involving phase change.

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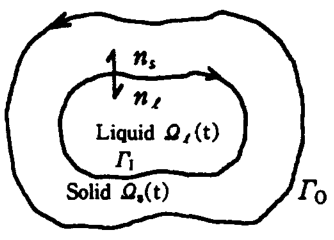

Fig. 1-a Geometrical model of the solidification problem

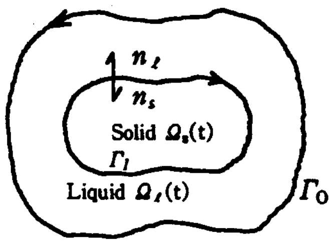

Fig. 1-b Geometrical model of the melting problem

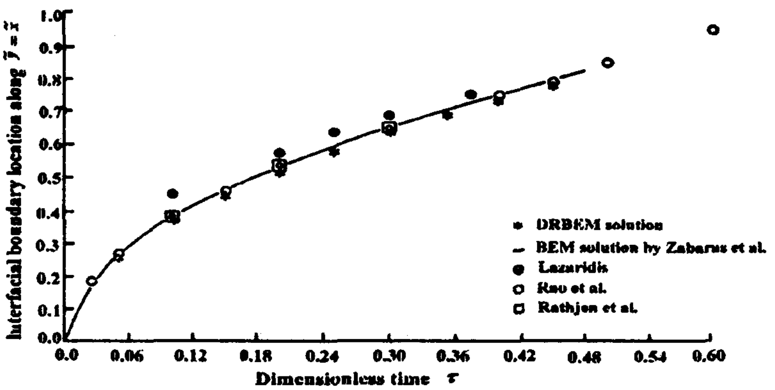

Fig. 2 Interfacial moving boundary motion along the diagonal $y = x$ as a function of timel.

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